iqtc

Institut de Química Teòrica i Computacional

EXCELENCIA MARÍA DE MAEZTU

UNIVERSITAT DE BARCELONA

Activity Report 2024

The creation of the Institute of Theoretical and Computational Chemistry of the *Universitat de Barcelona* (IQTCUB) was approved by the University's Government Council in an ordinary session on November 21st, 2007. From April 2018 I have the honor to serve as Director and I want to take the opportunity of being at the forefront of the IQTCUB's annual. Additionally, from the point of view of external recognition, the María de Maeztu awarding has allowed to incorporate new grant holders and postdocs into the Institute giving us an increase in the quality and quantity of our research. The year 2022 has meant an important consolidation of our Institute with the renewal of the María de Maeztu seal of excellence for four more years. Another important point has been the incorporation of senior researchers through programs like Beatriu de Pinós, Juan de la Cierva, Junior Group Leader La Caixa, Ramón y Cajal and ICREA.

The main goal of the research projects developed at the Institute is the use of quantum chemistry methods, although recently with the inclusion of experimental groups from our departments, new collaborations beyond Computational Chemistry have been initiated fostering and increasing the multidisciplinary character of our research. Traditionally, IQTC research is different from what everyone expects from a traditional chemist since the instrumentation used by our researchers is not located in a traditional laboratory but in a computational "laboratory" that is usually the gateway to our resources or to supercomputing centers with even greater computational capacity. A primary objective now is to enhance collaboration among the Institute's groups, especially the new incorporations that will contribute to strengthening the structure of the center.

Computational chemistry is in a period of profound change. The inclusion of methods based on Artificial Intelligence will mean a drastic change in the way of understanding Science, and in how to approach scientific challenges. In our Institute, many groups are currently using this type of tools, and this will provide new challenges and the ability to address more complex systems. Due to the availability in the short/medium term of quantum computers that will completely change our usual way of working. Within quantum computing, developing new computational methods that can take advantage of this new type of computers is crucial at this time. Thus, in 4-5 years' time, when computers with thousands of qubits will be available, it will be possible to study highly complex systems with a precision that is not possible with classical computers. This will represent an additional step forward in the studies that are currently being carried out. According to this, this field will provide new concepts that will allow progress in different aspects such as the rational design of new materials with specific physical properties and their application in electronics and magnetic devices; in the discovery of new drugs and in the understanding of the biochemical processes behind them; in new reactions that improve chemical processes to make them more efficient and environmentally friendly; and in the proposal of new sustainable energy sources to overcome the challenges facing our society today.

Eliseo Ruiz
Director of IQTCUB

IQTCUB OVERVIEW

The Institute of Theoretical and Computational Chemistry of the *Universitat de Barcelona* (IQTCUB), was created by the university Government Board on November 27th, 2007, with the main goal of enhancing and supporting scientific research in Theoretical and Computational Chemistry at the *Universitat de Barcelona* by organizing the research in four main lines and promoting and supporting interdisciplinary activities which will allow to tackle the new challenges in this scientific discipline.

Direction Team

The IQTCUB direction team during 2024 has been:

Prof. Eliseo Ruiz Sabin	*Director*
Prof. Francesc Viñes Solana	*Secretary*
Ms. Aïda Valverde	*Project Manager*

IQTCUB RESEARCH LINES

Scientific research currently being carried out at the IQTCUB can be viewed as classified in the following three main research lines.

1. **Catalysis, energy and environment**

What are the mechanisms of crucial chemical processes in energy conversion? Computational chemistry modelling can help in the design of new catalytic materials that can be crucial for electricity production in fuel-cell systems, as well as the catalysts involved in the activation of CO_2 and chemical or electrochemical conversion into useful molecules such as methane, ethylene or ethanol. Furthermore, theoretical approaches could also provide valuable insights into the mechanisms of the oil-water-rock interactions involved in the enhancement of oil recovery.

2. **Nanomaterials for emergent technologies**

Which chemical compounds exhibit the best magnetic or electron transport properties? The analysis through electronic structure methods provides an accurate understanding of the physical basis of these properties. The most promising molecular materials can include organic radicals, coordination compounds and 2D or 3D materials, that are technologically interesting due to their energy transfer, electronic and magnetic properties, in the search of multifunctional and switchable materials. Computational studies are extremely helpful to implement experiments with appealing targets to be synthesized.

3. Biocatalysis and drug discovery

What are the key molecular mechanisms in biological systems? Simulations involving thousands of atoms can be applied to model biomaterials and molecular mechanisms in biologically relevant molecules. Theoretical approach and the implementation of quantum chemistry and mechanical chemistry is useful to investigate the structure and reactivity of proteins and enzymes, to design new drugs, to describe processes in cellular membranes, enzymatic reactions in crowded media and soft nanoparticles in solution.

IQTCUB MEMBERS

IQTCUB involves more than 140 professors and researchers: The full list of members of IQTCUB (including the corresponding academic situation and affiliation within UB) is provided below.

Full Professors

Surname	Name	Country	Gender	Depart. Unit
Alemany i Canher	Pere	Spain	Male	Department of Materials Science and Physical Chemistry
Aullón López	Gabriel	Spain	Male	Department of Inorganic and Organic Chemistry
Bofill Villà	Josep Maria	Spain	Male	Department of Inorganic and Organic Chemistry
Curutchet Barat	Carles	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Deumal Solé	Mercè	Spain	Female	Department of Materials Science and Physical Chemistry
Giménez Font	Xavier	Spain	Male	Department of Materials Science and Physical Chemistry
González Pérez	Miguel	Spain	Male	Department of Materials Science and Physical Chemistry
Illas Riera	Francesc	Spain	Male	Department of Materials Science and Physical Chemistry
Llunell Marí	Miquel	Spain	Male	Department of Materials Science and Physical Chemistry
Lucas Alcorta	Josep Maria	Spain	Male	Department of Materials Science and Physical Chemistry
Luque Garriga	Francisco Javier	Spain	Male	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science

Mas Pujadas	Francesc	Spain	Male	Department of Materials Science and Physical Chemistry
Mota Valeri	Fernando	Spain	Male	Department of Materials Science and Physical Chemistry
Reigada Sanz	Ramon	Spain	Male	Department of Materials Science and Physical Chemistry
Ribeiro Moreira	Iberio de Pinho		Male	Department of Materials Science and Physical Chemistry
Rubio Martínez	Jaime	Spain	Male	Department of Materials Science and Physical Chemistry
Ruiz Sabin	Eliseo	Spain	Male	Department of Inorganic and Organic Chemistry
Sayós Ortega	Ramon	Spain	Male	Department of Materials Science and Physical Chemistry
Solé Sabaté	Albert	Spain	Male	Department of Materials Science and Physical Chemistry
Sousa Romero	María del Carmen	Spain	Female	Department of Materials Science and Physical Chemistry
Vilaseca Font	Eudald	Spain	Male	Department of Materials Science and Physical Chemistry

Aggregate Professors

Surname	Name	Country	Gender	Depart. Unit
Bonet Ruiz	Jordi	Spain	Male	Department of Chemical Engineering and Analytical Chemistry
Gamallo Belmonte	Pablo	Spain	Male	Department of Materials Science and Physical Chemistry
Huarte Larrañaga	Fermín	Spain	Male	Department of Materials Science and Physical Chemistry
Jover Modrego	Jesús	Spain	Male	Department of Inorganic and Organic Chemistry
Limburg	Bart	Holland	Male	Department of Inorganic and Organic Chemistry
Madurga Díez	Sergio	Spain	Male	Department of Materials Science and Physical Chemistry
Plesu Popescu	Alexandra	Spain	Female	Department of Chemical Engineering and Analytical Chemistry
Ribas Ariño	Jordi	Spain	Male	Department of Materials Science and Physical Chemistry

Viñes Solana	Francesc	Spain	Male	Department of Materials Science and Physical Chemistry

ICREA Research Professors

Surname	Name	Country	Gender	Depart. Unit
Bromley	Stefan		Male	Department of Materials Science and Physical Chemistry
Neyman	Konstantin M.	Germany	Male	Department of Materials Science and Physical Chemistry
Poater Teixidor	Jordi	Spain	Male	Department of Inorganic and Organic Chemistry
Puigmartí Luis	Josep	Spain	Male	Department of Materials Science and Physical Chemistry
Rovira Virgili	Carme	Spain	Female	Department of Inorganic and Organic Chemistry

Lecturer Professors

Surname	Name	Country	Gender	Depart. Unit
Cortijos Aragonès	Albert	Spain	Male	Department of Materials Science and Physical Chemistry
Estarellas Martín	Carolina	Spain	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Gómez Coca	Silvia	Spain	Female	Department of Inorganic and Organic Chemistry
Juárez Jiménez	Jordi	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Morales García	Ángel	Spain	Male	Department of Materials Science and Physical Chemistry
Sorrenti	Alessandro	Italy	Male	Department of Inorganic and Organic Chemistry

Postdoctoral Researchers

Contracte Projecte de Recerca

Surname	Name	Country	Gender	Depart. Unit
Corbella Morató	Marina	Spain	Female	Department of Inorganic and Organic Chemistry
Garcia Cirera	Beltzane	Spain	Female	Department of Materials Science and Physical Chemistry
Kapse	Samadhan	India	Male	Department of Materials Science and Physical Chemistry
Voccia	Maria	Italy	Female	Department of Materials Science and Physical Chemistry

Ramón y Cajal

Surname	Name	Country	Gender	Depart. Unit
Bruix Fusté	Albert	Spain	Male	Department of Materials Science and Physical Chemistry
Cirera Fernández	Jordi	Spain	Male	Department of Inorganic and Organic Chemistry
Fumanal Quintana	Maria	Spain	Female	Department of Materials Science and Physical Chemistry
Guix Noguera	Maria	Spain	Female	Department of Materials Science and Physical Chemistry
Kumar	Mohit	India	Male	Department of Inorganic and Organic Chemistry
Matheu	Roc	Spain	Male	Department of Inorganic and Organic Chemistry
Raich	Lluís	Spain	Male	Department of Inorganic and Organic Chemistry

Beatriu de Pinós-Juan de la Cierva

Surname	Name	Country	Gender	Depart. Unit
Mondal	Biswajit	India	Male	Department of Inorganic and Organic Chemistry

Marie-Curie

Surname	Name	Country	Gender	Depart. Unit
Liao	Qinghua	China	Male	Department of Inorganic and Organic Chemistry

Maria de Maeztu

Surname	Name	Country	Gender	Depart. Unit
Saletra	Wojciech		Male	Department of Inorganic and Organic Chemistry
Santiago Piera	Raúl	Spain	Male	Department of Materials Science and Physical Chemistry
Stasyuk	Anton	Russia	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Telari	Emanuele	Italy	Male	Department of Materials Science and Physical Chemistry

Others

Surname	Name	Country	Gender	Depart. Unit
Dmitriev	Igor		Male	Department of Inorganic and Organic Chemistry
Evans	Rhys	United Kingdom	Male	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science

Figueras	Marc	Spain	Male	Department of Materials Science and Physical Chemistry
Llabrés Prat	Salomé	Spain	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Ortiz Acero	Yenni	México	Female	Department of Materials Science and Physical Chemistry
Romanowska	Samanta		Female	Department of Inorganic and Organic Chemistry
Sharma	Poonam	India	Female	Department of Inorganic and Organic Chemistry

Predoctoral Researchers

FI Grant

Surname	Name	Country	Gender	Depart. Unit
Barmpidi	Katerina	Greece	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Betkhoshvili	Sergi	Georgia	Male	Department of Inorganic and Organic Chemistry
Blanco Gabella	Patricia	Spain	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Dolz García	Daniel	Spain	Male	Department of Materials Science and Physical Chemistry
García-Romeral González	Néstor Mauricio	Spain	Male	Department of Materials Science and Physical Chemistry
Llauradó Capdevila	Gemma	Spain	Female	Department of Materials Science and Physical Chemistry
Mariñoso Guiu	Joan		Male	Department of Materials Science and Physical Chemistry
Muriel Sánchez	Adrian		Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Özaydin	Gül Beste	Turkey	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Piniello Castillo	Beatriz	Spain	Female	Department of Inorganic and Organic Chemistry

FPI Grant

Surname	Name	Country	Gender	Depart. Unit
Allès Coll	Miquel	Spain	Male	Department of Materials Science and Physical Chemistry

Almacellas Salillas	David	Spain	Male	Department of Inorganic and Organic Chemistry
Atance	Pablo	Spain	Male	Department of Inorganic and Organic Chemistry
Calzada Escrig	Adrià	Spain	Male	Department of Materials Science and Physical Chemistry
Cánovas Montes	Manuel Antonio	Spain	Male	Department of Materials Science and Physical Chemistry
Castro Latorre	Pablo	Chile	Male	Department of Materials Science and Physical Chemistry
Cortés Llamas	Arnau	Spain	Male	Department of Materials Science and Physical Chemistry
Cuxart Sánchez	Irene	Spain	Female	Department of Inorganic and Organic Chemistry
Farris	Riccardo	Italia	Male	Department of Materials Science and Physical Chemistry
Garcia	Arnau	Spain	Male	Department of Inorganic and Organic Chemistry
Gómez Gordo	Mireia	Spain	Female	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Gómez Mudarra	Francisco Alonso	Spain	Male	Department of Inorganic and Organic Chemistry
Mamusi	Fatemeh	Spain	Female	Department of Materials Science and Physical Chemistry
Recio Poo	Miguel	Spain	Male	Department of Materials Science and Physical Chemistry
Regalado Aguilar	Mauricio	Spain	Male	Department of Inorganic and Organic Chemistry
Romeo	Eleonora	Italy	Female	Department of Materials Science and Physical Chemistry
Silvestre Llora	Adriana	Spain	Female	Department of Inorganic and Organic Chemistry
Vidal Gironès	Òscar	Spain	Male	Department of Inorganic and Organic Chemistry

FPU Grant

Surname	Name	Country	Gender	Depart. Unit
Orradre Altabás	Javier	Spain	Male	Department of Materials Science and Physical Chemistry

ITN UE Grant

Surname	Name	Country	Gender	Depart. Unit
Ergün	Özge	Turkey	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry

Ivanova	Varbina		Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry

UB/ADR Grant

Surname	Name	Country	Gender	Depart. Unit
Dias da Cunha	Renato	Brazil	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Jutglar Lozano	Kílian	Spain	Male	Department of Materials Science and Physical Chemistry
Martínez Medina	Yaiza	Spain	Female	Department of Inorganic and Organic Chemistry
Navarro Maestro	Laia	Spain	Female	Department of Inorganic and Organic Chemistry
Peralta Moreno	Maria Nuria	Spain	Female	Department of Materials Science and Physical Chemistry

Contracte Projecte de Recerca

Surname	Name	Country	Gender	Depart. Unit
Gonzalo Palao	Daniel	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry

J. E. Delima	David	Philippines	Male	Department of Inorganic and Organic Chemistry
Pepe	Alessandro	Italia	Male	Department of Inorganic and Organic Chemistry
Rivas Fernández	José Pablo	Spain	Male	Department of Inorganic and Organic Chemistry
Sağıroğlugil	Mert	Turkey	Male	Department of Inorganic and Organic Chemistry

Contracte Maria de Maeztu

Surname	Name	Country	Gender	Depart. Unit
Blas Buch	Daniel	Spain	Male	Department of Materials Science and Physical Chemistry
Clop	Oriol	Spain	Male	Department of Inorganic and Organic Chemistry
Colomer Llombart	Eduard	Spain	Male	Department of Materials Science and Physical Chemistry
Díaz Canals	Blanca	Spain	Female	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Franquesa	Pau	Spain	Male	Department of Materials Science and Physical Chemistry
Gracia Gil	Alejandro	Spain	Male	Department of Materials Science and Physical Chemistry
Rodríguez	Francesc Xavier	Spain	Male	Department of Inorganic and Organic Chemistry
Sánchez Muñoz	Laura	Spain	Female	Department of Materials Science and Physical Chemistry
Vidal Ramón	Daniel	Spain	Male	Department of Materials Science and Physical Chemistry

Others

Surname	Name	Country	Gender	Depart. Unit
Alsina Cowie	Marc	Spain	Male	Department of Inorganic and Organic Chemistry
Cabello Gallego	Ruben	Spain	Male	Department of Chemical Engineering and Analytical Chemistry
Cao	Wei	China	Male	Department of Materials Science and Physical Chemistry
Cardona Olives	Joan	Spain	Male	Department of Inorganic and Organic Chemistry
Casas	Carlota	Spain	Female	Department of Inorganic and Organic Chemistry

De Donato Pérez	Andreu Avel·lí	Spain	Male	Department of Materials Science and Physical Chemistry
De Moya Valenzuela	Natalia	Spain	Female	Department of Materials Science and Physical Chemistry
Distefano	Chiara	Italy	Female	Department of Inorganic and Organic Chemistry
Garcia Gonzalo	Lluc	Spain	Male	Department of Inorganic and Organic Chemistry
Herrera Restrepo	Ramón Santiago	Colombia	Male	Department of Materials Science and Physical Chemistry
Lleopart Motis	Genís		Male	Department of Materials Science and Physical Chemistry
Mazo Pirla	Laura Meiya		Female	Department of Inorganic and Organic Chemistry
Meng	Ling	China	Female	Department of Materials Science and Physical Chemistry
Morales Salvador	Raúl	Spain	Male	Department of Materials Science and Physical Chemistry
Ngo	Tuan	Vietnam	Male	Department of Materials Science and Physical Chemistry
Nguyen	Thao	Vietnam	Female	Department of Materials Science and Physical Chemistry
Ontiveros Cruz	Diego	Spain	Male	Department of Materials Science and Physical Chemistry
Quinlinvan Domínguez	Jon Eunan	Spain	Male	Department of Materials Science and Physical Chemistry
Serrano Morrás	Álvaro	Spain	Male	Department of Pharmacy and Pharmaceutical Technology, and Physical Chemistry
Solé Sabaté	Alex	Spain	Male	Department of Inorganic and Organic Chemistry
Troyano Ferré	Carles	Spain	Male	Department of Chemical Engineering and Analytical Chemistry
Valdivia Escribà	Aitor	Spain	Male	Department of Nutrition, Food Sciences and Gastronomy Basic Sciences Applied to Food Science
Vanrell Sabater	Antoni	Spain	Male	Department of Inorganic and Organic Chemistry

Vázquez Praga	David	Spain	Male	Department of Materials Science and Physical Chemistry
Venugopal	Akhil		Male	Department of Inorganic and Organic Chemistry

Research Technicians

Surname	Name	Country	Gender	Depart. Unit
Carvalho	David	Portugal	Male	Department of Materials Science and Physical Chemistry
Nicholas	James	United Kingdom	Male	Department of Materials Science and Physical Chemistry
Noori	Zahra	Iran	Female	Department of Materials Science and Physical Chemistry
Romo	Marc	Spain	Male	Department of Inorganic and Organic Chemistry

Technical staff

Apart from the academic and research personnel whose main activity is scientific research in theoretical and computational chemistry at IQTCUB, technical staff members take care of maintenance of the computational infrastructure and give support to the research groups. Their work is extremely important since they also implement the codes and optimize their performance.

Jordi Inglés Camats	*HPC System Administrator Manager*
Irene Zamora Carretero	*HPC System Administrator*
Jhonathan Rosa de Souza	Research Technician
Aïda Valverde Sanchís	*Project Manager and Promoter*

Equipment

Currently, the IQTCUB computational facilities consist of nine calculation clusters located in two conditioned rooms of the Chemistry and Physics Faculty of UB. All the clusters except iqtc06 and iqtc07 are in a room near the garage of the faculty where it is cooled by two air conditioning machines of 47,000 and 66,000 KW, respectively. Iqtc06 and iqtc07 are located in a room called VAX, which is cooled by one air conditioner machine of 30,000 KW and another two of 9,000KW each.

Calculation clusters

iqtc04 (*invested value 460.000 €*)

Machine type	HP cluster
Operating system	SLES11
Services	Calculation cluster
Structure	101 nodes
Notes	64 bits processors. Infiniband network

Specifications:

95 INTEL HP ProLiant DL160 G6 nodes
CPU: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (internal data network) + 2 infiniband network (calculation network) + 1 ILO card (IAM)

4 INTEL HP ProLiant DL160 G6 nodes
CPU: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 4 x 500 GB hard disk
Network: 2 gigabit network card (internal data network and calculation network) + 1 ILO card (OOB)

2 INTEL HP ProLiant DL160 G6 nodes
CPU: 2 x 2,66 GHz Xeon SixCore RAM: 48 GB
HD: 1 x 500 GB hard disk
Network: 2 gigabit network card (internal data network and calculation network) + 1 ILO card (OOB)

iqtc06 (*invested value 420.000 €*)

Machine type	Heterogeneous Cluster
Operating System	SLES11
Services	Calculation cluster
Structure	32 nodes
Notes	64 bits processors

Specifications:

25 INTEL HP ProLiant DL560 Gen8 nodes
CPU: 4 x 2,2 GHz Xeon OctoCore
RAM: 512 GB
HD: 2 x 300 GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10 gigabit network card (internal data network)

7 INTEL Supermicro SuperServer 8017R-TF+
CPU: 4 x 2,3 GHz Xeon OctoCore
RAM: 512 GB
HD: 3 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

iqtc07 (*invested value 40.000 €*)

Machine type	Supermicro Cluster
Operating System	SLES12
Services	Calculation cluster
Structure	2 nodes
Notes	64 bits processors

Specifications:

2 Supermicro 2048U RT4 nodes
CPU: 4 x 2,6 GHZ Intel Broadwell 10Core
RAM: 512 GB or 1 TB
HD: 1 x 1 TB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

iqtc08 (*invested value 175.000 €*)

Machine type	HP Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	22 nodes
Notes	64 bits processors

Specifications

22 HP Proliant DL360 Gen9
CPU: 2 x 2,6 GHz Intel Xeon E5-2690 v4 14-core
RAM: 768 GB
HD: 1 x 1 TB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
Network: 2 x 10gigabit network card (internal data network)

iqtc09 (*invested value 340.000 €*)

Machine type	Gigabyte Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	30 nodes
Notes	64 bits processors

Specifications

26 Gigabyte R13
CPU: 2 x 2,9 GHz AMD EPYC 7542 32-core processor (64 cores)
RAM: 1 TB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

4 Gigabyte R182
CPU: 2 x 2,3 GHz AMD EPYC 7642 48-core processor (96 cores)
RAM: 1 TB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

lqtc10 (*invested value 244.000 €*)

Machine type	Gigabyte Cluster
Operating System	Centos 7.2
Services	Calculation cluster
Structure	13 nodes (32 GPU RTX 3090, 8 RTX3080)
Notes	64 bits processors

Specifications

5 Gigabyte G482-Z54-00
CPU: 2 x 3,0 GHz AMD EPYC 7313 16-core processor (32 cores)
RAM: 128 GB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card
GPU: 4 x RTX3090 NVIDIA

3 Gigabyte G292-Z44-00
CPU: 2 x 2.8 GHz AMD EPYC 7282 16-core processor (32 cores)
RAM: 256 GB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card
GPU: 4 x RTX3090 NVIDIA

3 Gigabyte G482-Z54-00
CPU: 2 x 2.8 GHz AMD EPYC 7282 16-core processor (32 cores)
RAM: 256 GB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card
GPU: 8 x RTX3080 NVIDIA

2 Gigabyte G482-Z54-00
CPU: 2 x 3 GHz AMD EPYC 7313 16-core processor (32 cores)
RAM: 256 GB
HD: 1 x 8 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card
GPU: 8 x RTX3090 NVIDIA

lqtc11 (*invested value 100.000 €*)

Machine type Gigabyte Cluster
Operating System Centos 7.2
Services Calculation cluster
Structure 9 nodes + 1 file server
Notes 64 bits processors

Specifications

9 Gigabyte R182-340-00
CPU: 2 x 2.80GHz Intel Xen Plantium 8362 32-core processor (64 cores) RAM: 1 TB
HD: 1 x 2 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

1 Gigabyte R282-3C1-00
CPU: 2 x 2.60Ghz Intel Xen Plantium 8358 32-core processor (64 cores) RAM: 128 GB
HD: 100 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

Iqtc12 (*invested value 220.750 €*)

Machine type Supermicro & Gigabyte Cluster
Operating System Rocky Linux 8.8
Services Calculation cluster
Structure 10 nodes
Notes 64 bits processors, Multi-Core, HyperThreading
Specifications

8 Supermicro AS-2025HS-TNR
CPU: 2 x 3.10GHz AMD EPYC 9554 64-Core Processor (128 cores) RAM: 3 TB
HD: 1 x 30 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

2 Gigabyte R282-3C1-00
CPU: 2 x 2.60Ghz Intel Xen Plantium 8358 32-core processor (128 cores) RAM: 755.1 GB
HD: 7.3 TB SATA hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (internal administration network) + 2 x 10 GB network card

GPU cluster (*invested value 75.000 €*)

Machine type	Heterogeneous Cluster
Operating System	SLES11, centos 7
Services	Calculation cluster with GPUs
Structure	*5* nodes
Notes	64 bits processors

Specifications:

Node

CPU: 1 x 3,06 GHz Intel Core i7 950
RAM: 16 GB
HD: 1 x 1 TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX580, 1 NVIDIA GTX480

Node Tyan FT72B7015

CPU: 2 x 2,66 GHz Xeon SixCore
RAM: 48 GB
HD: 1 x 500 GB hard disk
Network: 4 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 8 NVIDIA GTX580

Node

CPU: 1 x 3,30 GHz AMD FX-4100 QuadCore
RAM: 16 GB
HD: 1 x 1 TB hard disk
Network: 1 gigabit network card (calculation network)
GPU: 1 NVIDIA GTX770

Node ASUS ESC4000 G2

CPU: 2 x 2 GHz Xeon SixCore
RAM: 32 GB
HD: 1 x 2 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX TITAN

Node ASUS ESC4000 G2

CPU: 2 x 2,4 GHz Xeon SixCore
RAM: 32 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX TITAN BLACK

Node AZServer 4G3S

CPU: 2 x 2,4 GHz Xeon E5-2620v3
RAM: 32 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 4 NVIDIA GTX 980

Node SIE LADON BROADWELL
CPU: 2 x 2,4 GHz Xeon E5-2640v4
RAM: 128 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB) GPU: 4 NVIDIA TESLA K40

Node SIE LADON BROADWELL 2
CPU: 2 x 2,4 GHz Xeon E5-2640v4
RAM: 128 GB
HD: 1 x 1 TB hard disk
Network: 2 gigabit network card (calculation network) + 1 IPMI card (OOB)
GPU: 2 NVIDIA TESLA P100

2 Nodes AZServer 4G3S
CPU: 2 x 2,2 GHz Dual Xeon E5-2600v4 (10 cores)
RAM: 128 GB
HD: 2 x 2 TB hard disk
Network: 4 gigabit network card + 1 IPMI card (OOB)
GPU: 4 NVIDIA GEFORCE GTX 1070Ti

Servers

Disk server (*invested value 84.000 €*)

Machine type	HP cluster
Operating system	SLES 11
Services	Storage service cluster with 32TB of space for user's data exported by GlusterFS
Structure	2 nodes
Notes	Storage service with a dedicated UPS and redundant power supply

Specifications:

1 INTEL HP ProLiant DL180 G6 node CPU: 2 x 2,27 GHz Xeon QuadCore E5520 RAM: 56 GB
HD: 12 x 2 TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

1 INTEL HP ProLiant DL380e Gen8 node CPU: 2 x 2,20 GHz Xeon QuadCore E5-2407 RAM: 48 GB
HD: 12 x 2 TB (raid 5)
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

Machine type Supermicro
Operating system Centos 7.6

Services Storage service cluster with 64TB of space for applications directories and user's work area exported by NFS
Structure 1 node
Notes Storage service redundant power supply
Specifications:

1 Node Supermicro 2U
CPU: 2 x 2,20 GHz Xeon 4210
RAM: 64 GB
HD: 8 x 8 TB (raid 5)
Network: 4 gigabit network card
Network: 2 10GB network card

Machine type DELL
Operating system Centos 7.6
Services Storage service cluster with 100TB of space for applications directories and user's work area exported by GlusterFS
Structure 1 node
Notes Storage service redundant power supply

Specifications:

1 PowerEdge R740XD
CPU: 2 x 2,10 GHz Xeon 4110
RAM: 64 GB
HD: 10 x 10 TB (raid 5)
Network: 4 gigabit network card
Network: 2 10GB network card

Machine type	Supermicro
Operating system	Ubuntu Server 20.04
Services	Storage service cluster with 80TB of space for backup purposes
Structure	1 node
Notes	Storage service redundant power supply

Specifications:

1 Node Supermicro 2U

CPU: 4 x 2,40 GHz Xeon Silver 4314 (64 cores)

RAM: 128 GB

HD: 8 x 10 TB (raid 5)

Network: 2 10GB network card

Machine type	Supermicro
Operating system	Ubuntu Server 24.04
Services	Storage service cluster with 215TB of space for applications directories and user's work area exported by NFS
Structure	1 node
Notes	Storage service redundant power supply

Specifications:

1 Node Supermicro 2U
CPU: 4 x 2,10 GHz Xeon Silver 4310 (12 cores)
RAM: 256 GB

Portal (user access servers) (*invested value 4.500 €*)

Machine type	Portal access servers
Operating system	Debian stable / Debian 10.5
Services	SGE Execution Host, Heartbeat, ssh server
Structure	3 nodes
Notes	User access servers for submitting jobs and accessing user data. Critical service connected with a UPS

Specifications:

2 INTEL HP ProLiant DL120 G5 node
CPU: 1 x 2,33 GHz Xeon Dual Core
RAM: 8 GB
HD: 1 x 160 GB hard disk
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

1 DELL Poweredge R640 node
CPU: 1 x 2,2 GHz Xeon Silver 4210
RAM: 16 GB
HD: 1 x 256 GB hard disk
Network: 2 gigabit network card (internal network) + 1 IPMI card (OOB)

Virtualization servers (*invested value 28.300 €*)

Machine type	4 redundant nodes
Operating system	Debian stable
Services	Xen, DRBD, IQTCUB internal services
Structure	4 redundant nodes
Notes	Servers that contains the Xen virtual machines with the IQTCUB's internal services (SGE, dhcp, license server, etc.). Critical service connected with a UPS

Specifications:

2 INTEL DELL PowerEdge 2950 nodes
CPU: 2 x 2,50 GHz Xeon QuadCore E5420
RAM: 8 GB
HD: 2 x 1 TB (raid 1)
Network: 3 gigabit network card (internal network)

2 INTEL HP ProLiant DL120 G5 node
CPU: 1 x 2,33 GHz Xeon Dual Core
RAM: 8 GB
HD: 2 x 160 GB hard disk
Network: 3 gigabit network cards (internal network)

Machine type	1 node
Operating system	Centos 7.3
Services	Pre-production and testing proposals
Structure	1 node

Specifications:

1 DELL PowerEdge R640
CPU: 2 x 2 GHz Xeon Gold 6138
RAM: 128 GB
HD: 2 x 2 TB (raid 1)
Network: 2 gigabit network card + iDrac

Graphical applications server (*invested value 3.000 €*)

Machine type	1 HP ProLiant DL385 node
Operating system	Debian Stable
Services	Server for the use of graphical applications (gaussview, p4vasp, etc.)
Structure	1 node
Notes	Server connected to an UPS

Specifications:

1 AMD HP ProLiant DL385 node

CPU: 2 x 2,2 GHz AMD Opteron 275 Dualcore RAM: 4 GBHD: 6 x 146 GB hard disk Network:1 10/100 network (external network) + 1 gigabit network (internal network)

Others

The IQTCUB have other services to provide service to the IQTCUB's users.

1. Backup server DELL R515 (backup server with 4TB of disk capacity connected to a UPS).
2. Tape library server HP MSL4048 (48 tapes with approximately 144TB of space, ~3TB/tape).
3. Administration server (laptop with 3 network cards for critical incidences support).
4. Proxy server (server that allows the access to the public network from IQTCUB's network).
5. Switch Layer 3 HP Procurve with 24 ports (used for the IQTCUB's date centre infrastructure).
6. 8 Switchs Layer 2 Dlink with 48 ports (internal network for cerqt2, iqtc01, iqtc02, iqtc03 clusters).
7. 4 Switchs Layer 2 HP with 48 ports (internal network for iqtc04, iqtc05 and iqtc06 cluster).
8. 3 Switchs Infiniband Voltaire with 36 ports (calculation network for iqtc04 cluster).
9. Modular switch HP (8 calculation network modules for iqtc01, iqtc02, iqtc03 clusters).
10. 2 Modular switch HP 10GB (calculation network for iqtc06 and data network for the glusterfs servers).
11. 2 Switch Netgear XS728T 10GB (internal and calculation network for iqtc08).
12. 1 Switch HPE 1810-24 (internal network iqtc08).
13. 1 MSI LAPTOP with Oculus RIFT S -Virtual Reality Study-.
14. 1 XYZ printing da Vinci Color AIO 3D printer
15. 6 Oculus Quest

The approximate cost of this equipment is *58.000 €.*

Summary

Cores .....7,716 c

Memory.....96,117 GB RAM

Calculation disk capacity..... 336 TB

Data user disk capacity..... 215 TB

The amount invested, considering also the consumables such as network cables and other material is approximately.

*2.100.000 €**

*This value does not include the cost of the air conditioning machines and electrical panels.

IQTCUB ACTIVITIES

General Activities (courses, grants and dissemination)

Next, a description of activities and actions promoted by IQTCUB through 2024 is provided.

a. ***Molecular Modelling: biomolecules and drug design 2024.*** From February 6th to 9th, the summer computational school titled *Molecular Modelling: biomolecules and drug design 2024 took place.* Prof. Sergio Madurga and Prof. Jaime Rubio organized the event. In this edition, the sessions were given by the following researchers:

   - Analysis of non-covalent interactions in DNA base pairs. (Jordi Poater)
   - Simulation of macromolecular systems (Sergio Madurga)
   - Protein Molecular Dynamics (Carolina Estarellas and Salomé Llabrés)
   - Visualising biomolecules in action (Matín Calvelo and José Pablo Rivas)
   - Coarse-grained Molecular Dynamics simulations for soft-matter systems: from micelles to membranes (Ramón Reigada)
   - Drug Design (Jaime Rubio)
   - Multi-scale modelling of solutions and biomolecules (Carles Curutchet)

b. Computational Modelling: from Molecules to Materials 2024. From February 12th to 16th, the summer computational school titled *Computational Modelling: from Molecules to Materials 2024* took place. The organizers were Dr. Silvia Gómez and Prof. Gabriel Aullón. In this edition, the sessions were given by the following researchers:

   - Linux (Jordi Inglés and Irene Zamora)
   - Linkage and structure (Gabriel Aullón and Silvia Gómez)
   - Excited States (Mercè Deumal)
   - Molecular Reactivity (Jesús Jover)
   - Molecular dynamics (Miguel González)
   - Virtual reality in chemistry (Jordi Cirera)
   - Nanoclusters and Nanostructures Materials (Stefan Bromley)
   - Band Theory (Eliseo Ruiz)
   - Surfaces and defects (Ángel Morales)
   - Machine Learning (Albert Bruix)

c. ***IX Festa de la Ciència.*** The IQTC paticipated with the "Explora el món molecular en un entorn de realitat virtual" workshop. It took place on May 10th and 11th.

d. **Mini-symposium on Materials and Catalysis: Experiments and Modelling:** This mini-symposium took place on November 20th, 2024. The speakers were Prof. Paul Bagus (Center for Advanced Scientific Computing and Modelling, Univesity of North Texas, USA), Dr. José Rodríguez (Brookhaven National Laboratory, USA), Dr. Sergey Kozlov (National Univesity of Singapore, Singapore), and Prof. Karsten Reuter (Fritz-Haber-Institut der Max-Planck-Gesellschaft, Germany).

e. **Active nano/microsystems in the Spanish context:** This symposium focuses on both fundamental and applied studies of active microsystems, aiming to foster networking opportunities and collaboration within Spanish groups, as well as promote and advance our research internationally. It took place on October 24th and 25th, 2024, and the program included several researchers established in Spain, from universities like Universidad Complutense de Madrid, Universidad de Alcalá, and Universidad de Zaragoza, and institutes like Institut Català d'Investigació Química and Instituto de Bioingeniería de Cataluña.

f. **Twins in Catalysis: Merging Theory and Experiment:** This congress took place on November 21st and 22nd, 2024, and was co-organized with the Università degli Studi di Milano Bicocca. The speakers for this event were Prof. Livia Giordano (Università degli Studi di Milano Bicocca, Italy), Prof. Hans J. Freund (Fritz Haber Institute of the Max Planck Society, Germany), Prof. Paul Bagus (Center for Advanced Scientific Computing and Modelling, Univesity of North Texas, USA), Prof. Richard Catlow (University of Cardiff, United Kingdom), Dr. José Rodríguez (Brookhaven National Laboratory, USA), Dr. Verónica Ganduglia-Pirovano (Instituto de Catálisis y Petroleoquímica, Spain), Prof. Alexander Shluger University College London, United Kingdom), Prof. Josep M. Ricart (Universitat Rovira i Virgili, Spain), Prof. Nino Russo (University of Calabria, Italy), and Dr. Paola Luches (Istituto Nanoscienze, Italy).

g. **IQTC Meeting 2024:** The event took place on October 30th and 31st, intending to broaden views on topics of interest to our members. The two international invited speakers were Prof. Georg Kresse (Universität Wien, Austria) and Prof. Johannes Gierschner (Universitat de València, Spain).

IQTCUB Seminars and Conferences

During 2024 IQTC has organized the following seminars and conferences:

Dr. David Balcells (Hylleraas Centre of Excelence for Quantum Molecular Sciences, University of Oslo)
Machine Learning for Transition Metal Complexes: Deterministic, Evolutionary and Variational.
February 12th 2024

Prof. Dr. Martin Kaupp (Technische Universität Berlin)
New DFT Approaches Beyond the Zero-Sum Game and More.
March 12th 2024

Dr. Julian Fuchs (Boehringer Ingelheim)
Oprimizing Molecular Conformations and Interactions for Drug Design.
March 22th 2024

Prof. Maria Joao Ramos (University of Oporto)
Studies on Enzyme-Catalysed Reactions.
April 2nd 2024

Prof. Alessandra Magistrato (National Research Council-Institute of Material Foundry , Scuola Internazionale Superiore di Studi Avanzati)
All-Atom Simulations to Unravel Biomolecular Mechanisms: from pre-mRNA Splicing to Metal Ions Transport.
April 23rd 2024

Dr. Carlos Franco (Institute of Robotics and Intelligent Systems)
The Evolution and Innovation in Reticular Chemical Exploring MOFs and COFs from Concept to Process
May 27th 2024

Prof. Srecko Kirin (Ruder Boskovic Institute)
Transition Metal Complexes: Supramolecular Chemistry and Catalysis
May 24th 2024

Prof. Fahmi Himo (Stockholm Univesity)
Modeling Reactions in Enxymes and in Confined Spaces
June 10th 2024

Prof. Jaakko Akola (Norwegian University of Science and Technology)
Reaction Path Modelling of Hydrogen Evolution Reaction on MoS_2: Voltage and Solution Effects
June 17th 2024

Dr. Emanuele Telari (Sapienza Università di Roma)
Deep Collective Variables for Metal Nanoclusters Structural Transition
October 17th 2024

Prof. Darío Estrin (University of Buenos Aires and National Research Council)
Multi Scale Quantum-Classical (QM-MM) Simulation Schemes: Basics and Applications
November 12th 2024

IQTCUB Invited Researchers

Prof. Dr. Ma. Guadalupe Moreno Armenta (invited researcher)
National Autonomous University of Mexico, Mexico
February 2023–February 2024

Prof. Jaakko Akola (invited visitor)
Norwegian University of Science and Technology - NTNU, Norway
August 2023 to July 2024 and November 2024 (10 days)

Dr. Haruna L. Bararzorda (invted visitor)
Universidad Católica Santa María, Arequipa (Perú)
January-March, 2024

Prof. Hou Jianhua (invited researcher)
Changchun University of Science and Technology, China
December 2023–December 2024

Prof. Yongpeng Yang (invited researcher)
Zhengzhou University, China
January 2024–January 2025

Dr Julilen Fuchs (invited visitor)
Boheringer-Ingelheim, Austria
Jan-March 2024

Prof. William J. Zamora (invited visitor)
University of Costa Rica, Costa Rica
February 2024

Mrs. Somia Benchikh (research stay with Prof. Pablo Gamallo)
University of Setif, Algeria
Feb-Apr 2024

Prof. Jingli Han (invited visitor professor)
School of Material and Chemical Engineering, Zhengzhou University of Light Industry Zhengzhou, 450001, China
April/2024 - March/2025 (12 months)

Mrs. Javiera del Pilar Herrera Escalona (research stay with Prof. Pablo Gamallo)
Universidad de Concepción, Chile
Apr-June 2024

Mr. Luke di Liddo (research stay with Prof. Pablo Gamallo)
University of Toronto, Canada
May-June 2024

Dr Antonia Mey (invited visitor)
The Univeristy of Edinburgh, The United Kingdom
June 2024

Prof. Iskra Koleva (invited researcher)
University of Sofia, Bulgaria
July 2024

MSc. Bayan Karapenchev (invited researcher)
University of Sofia, Bulgaria
July 2024

Prof. Hristiyan A. Aleksandrov (invited visitor)
University of Sofia, Bulgaria
July, November 2024

Prof. Darío E. Estrín (invited visitor)
University of Buenos Aires, Argentina
September 2024

Prof. Benjamin Beck (invited visitor)
University of Brusselles, Belgium
September 2024

MSc. Ricardo Bermeo Campos (invited researcher)
National Politechnical Institute, Mexico
September–December 2024

Prof. Dr. Kyoung Chul Ko (invited researcher)
Chonnam National University, Korea
September 2024–September 2025

Prof. Cong Wang (invited researcher)
Changchun University of Science and Technology, China
October 2024–October 2025

Prof. Petr Jureča (invited visitor) Palacký
University Olomouc, Czech Republic
November 2024

Prof. Marie Zgarbová (invited visitor) Palacký
University Olomouc, Czech Republic
November 2024

Prof. Ciro Achille Guido (invited visitor)
Università del Piemonte Orientale, Italy
November 2024

Prof. Jose A. Rodriguez (invited researcher)
Brookhaven National Laboratory, US
November 2024

Prof. Dr. Paul S. Bagus (invited researcher)
University of North Texas, US
November 2024

Scientific Activity of IQTCUB Members
Highlights from the most Relevant Results

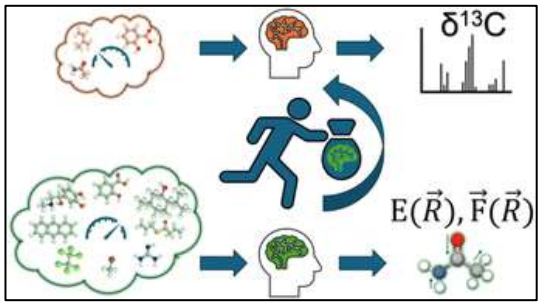
Here some of the most relevant results corresponding to every IQTCUB main research line are presented.

Line 1. Catalysis, energy, and environment

Transfer learning based on atomic feature extraction for the prediction of experimental ^{13}C chemical shifts

Ž. Ivković, J. Jover, J. N. Harvey

Digital Discovery, *3* (2024) 2242.



In this work we use transfer learning techniques to estimate experimental ^{13}C shifts of organic compounds with greater accuracy than previous studies, including DFT calculations and other ML tools. We found that atomic features from a message passing neural network (MPNN) forcefield are robust descriptors for atomic properties. A dense network using these descriptors achieves a mean absolute error (MAE) of 1.68 ppm, while a graph neural network (GNN) using these features achieves a better MAE of 1.34 ppm. Embeddings from a self-supervised pre-trained 3D aware transformer show reasonable accuracy within the GNN framework, achieving MAE of 1.51 ppm. Under low-data conditions, all transfer-learned models significantly improve predictive accuracy compared to existing models. Extracting atomic features from models trained on large datasets is effective for predicting NMR chemical shifts, offering benefits like reduced training times, simpler models, and strong performance in low-data scenarios. This technique can be applied to other chemical tasks, opening new applications where data is limited.

LNG Cold Energy Recovery for Hydrogen Production Combining Multiple Technologies in Synergy.

C.T. Ferré, R. Cabello, L.M. Marin, A. Plesu, J. Bonet, J. Llorens

Chemical Engineering Transactions, *114* (2024) 607–612.

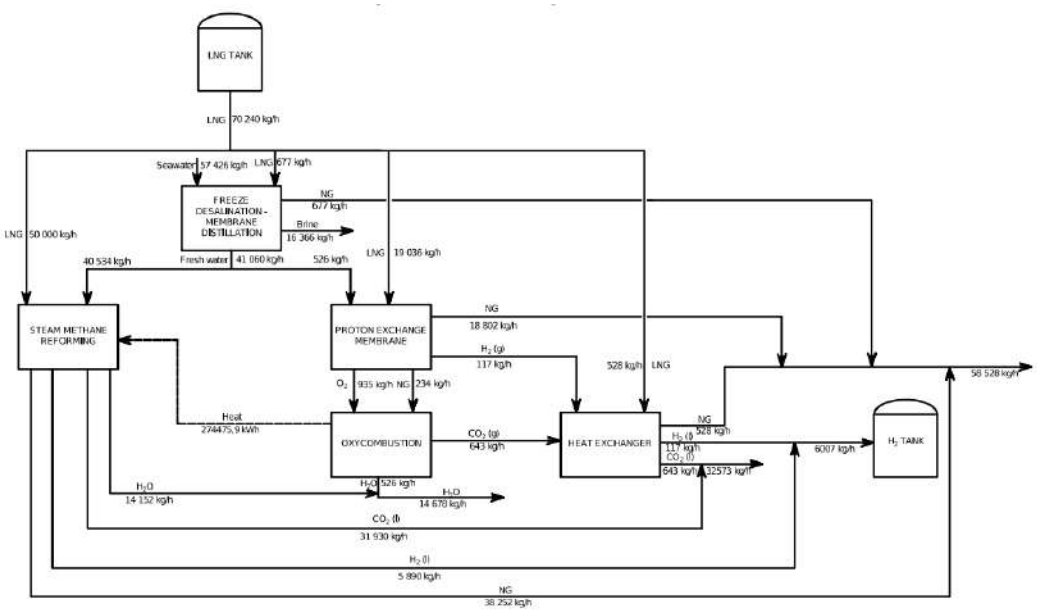


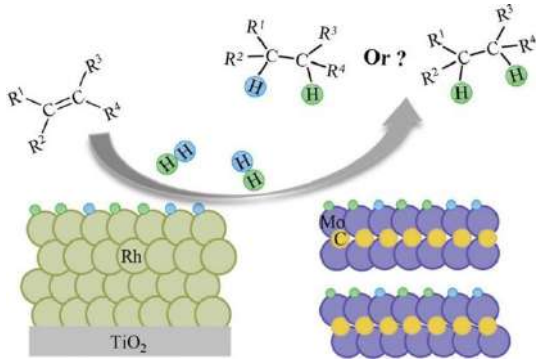
Figure. Details of the figure (optional).

A bibliographic search for levering the of cold energy of natural gas that arrives líquid via boat and it is proposed how to combine diferent options in sinergy to lever this cold energy to produce hydrogen.

Contrasting Metallic (Rh^0) and Carbidic (2D-Mo_2C MXene) Surfaces in Olefin Hydrogentaion Provides Insights on the Origin of the Pairwise Hydrogen Addition

L. Meng, E. V. Pokochueva, Z. Chen, A. Federov, F. Viñes, F.Illas, I. V. Koptyug

ACS Catal., *14* (2024) 12500-12511.



Kinetic studies are vital for gathering mechanistic insights into heterogeneously catalyzed hydrogenation of unsaturated organic compounds (olefins), where the Horiuti–Polanyi mechanism is ubiquitous on metal catalysts. While this mechanism envisions nonpairwise H_2 addition due to the rapid scrambling of surface hydride (H*) species, a pairwise H_2 addition is experimentally encountered, rationalized here based on density functional theory (DFT) simulations for the ethene (C_2H_4) hydrogenation catalyzed by two-dimensional (2D) MXene $Mo_2C(0001)$ surface and compared to Rh(111) surface. Results show that ethyl (C_2H_5*) hydrogenation is the rate-determining step (RDS) on $Mo_2C(0001)$, yet C_2H_5* formation is the RDS on Rh(111), which features a higher reaction rate and contribution from pairwise H_2 addition compared to 2D-$Mo_2C(0001)$. This qualitatively agrees with the experimental results for propene hydrogenation with parahydrogen over 2D-Mo_2C_{1-x} MXene and Rh/TiO_2. However, DFT results imply that pairwise selectivity should be negligible owing to the facile H* diffusion on both surfaces, not affected by H* nor C_2H_4* coverages. DFT results also rule out the Eley–Rideal mechanism appreciably contributing to pairwise addition. The measurable contribution of the pairwise hydrogenation pathway operating concurrently with the dominant nonpairwise one is proposed to be due to the dynamic site blocking at higher adsorbate coverages or another mechanism that would drastically limit the diffusion of H* adatoms.

Electrostatic catalysis of a click reaction in a microfluidic cell

Semih Sevim, Roger Sanchis-Gual, Carlos Franco, Albert C. Aragonès, Nadim Darwish, Donghoon Kim, Rosaria Anna Picca, Bradley J. Nelson, Eliseo Ruiz, Salvador Pané*, Ismael Díez-Pérez*, Josep Puigmartí-Luis*

Nature Communications, *15*, (2024) 790.

Fig. 1: Catalysis of a click reaction in a microfluidic cell.

From: Electrostatic catalysis of a click reaction in a microfluidic cell

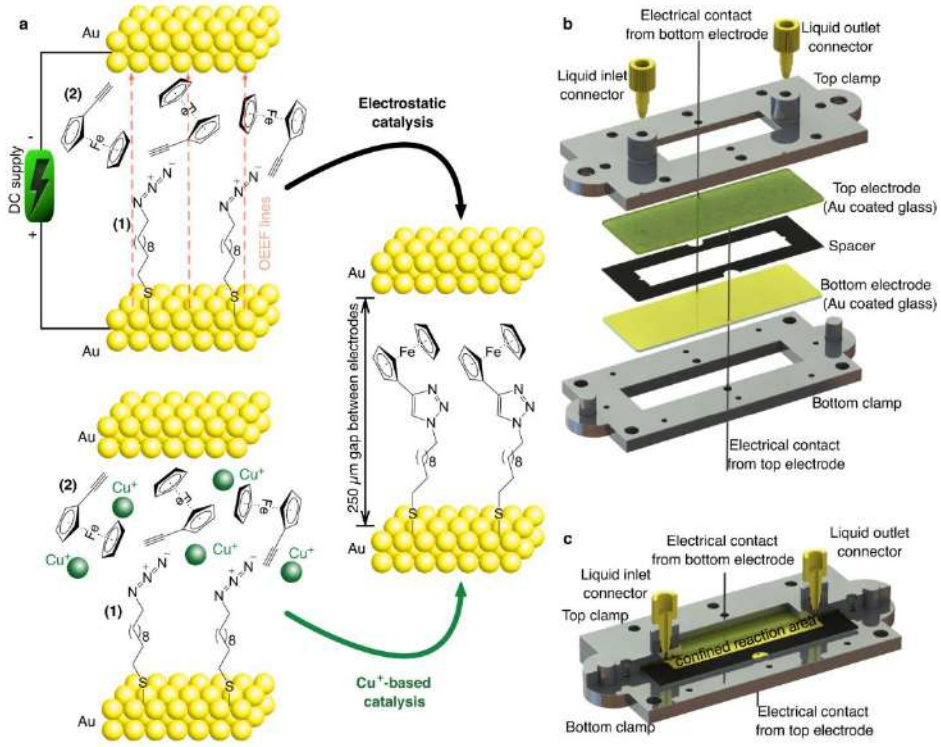
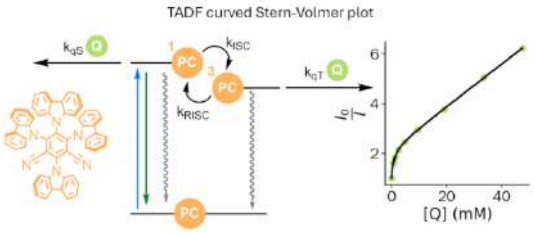


Figure. Schematic representation of oriented external electric-field (OEEF) in an electrostatic catalysis (top panel), and copper (Cu^+)-catalyzed click cycloaddition (bottom panel) in a confined microfluidic channel between two gold electrodes.

Electric fields can directly trigger or accelerate chemical processes with stereo- and regio-specificity. In enzymatic catalysis, controlled mass transport of chemical species is also key in facilitating the availability of reactants in the active reaction site. Recent progress in developing a clean catalysis that profits from oriented electric fields is limited to theoretical and experimental studies at the single molecule level, where control over mass transport and scalability cannot be tested. Here, we quantify the electrostatic catalysis of a prototypical Huisgen cycloaddition in a large-area electrode surface and directly compare its performance to the conventional Cu(I) catalysis. Our microfluidic cell enhances reagent transport towards the electrified reactive interface. This continuous-flow microfluidic electrostatic reactor is an example of an electric-field driven platform where clean large-scale electrostatic catalytic processes can be efficiently implemented and regulated.

An Extension of the Stern–Volmer Equation for Thermally Activated Delayed Fluorescence (TADF) Photocatalysts

B Limburg. *J. Phys. Chem. Lett.* **2024**, *15*, 10495-10499

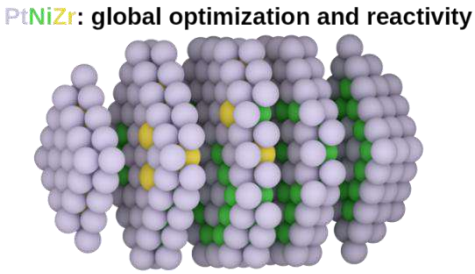


Fluorescence quenching experiments are essential mechanistic tools in photoredox catalysis, allowing one to elucidate the first step in the catalytic cycle that occurs after photon absorption. Thermally activated delayed fluorescence (TADF) photocatalysts, however, yield nonlinear Stern–Volmer plots, thus requiring an adjustment to this widely used method to determine the efficiency of excited state quenching. Here, we derive an extension of the Stern–Volmer equation for TADF fluorophores that considers quenching from both the singlet and triplet excited states and experimentally verify it with fluorescence quenching experiments using the commonly employed TADF-photocatalyst 4CzIPN, and multiple-resonance TADF-photocatalyst QAO with three different quenchers in four solvents. The experimental data are perfectly described by this new equation, which in addition to the Stern–Volmer quenching constants allows for the determination of the product of intersystem and reverse intersystem crossing quantum yields, a quantity that is independent of the quencher.

Effects of Zr dopants on properties of PtNi nanoparticles for ORR catalysis: a DFT modeling.

R. Farris, B.V. Merinov, A. Bruix, K.M. Neyman.

J. Chem. Phys., *160* (2024) 124706.

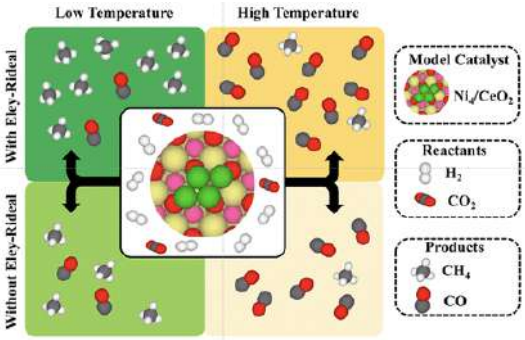


Pt-based alloys are among the best electrocatalysts for oxygen reduction reaction (ORR) in polymer electrolyte membrane fuel cells. Doping of PtNi alloys with Zr enhances the durability of the operating ORR catalysts. This study aimed at understanding the structure-property relations in Zr-doped PtNi nanoparticles (NPs) as a key to their ORR function. Using a method based on Density Functional Theory, the most stable chemical orderings of pristine and Zr-doped Pt_3Ni NPs containing over 400 atoms were calculated to clarify: *i*) preferential location and charge states of Zr atoms in the Pt_3Ni NPs; *ii*) effect of doping Zr atoms on the stability of the Pt skin of the Pt_3Ni NPs; *iii*) charge redistribution induced by Zr dopants; *iv*) layer-by-layer atomic ordering in the Pt_3Ni/Zr NPs with increasing Zr content; and *v*) effect of Zr atoms on the adsorption energies of O and OH species as indicators of the ORR activity.

Comprehensive Density Functional and kinetic Monte Carlo Study of CO_2 Hydrogenation on a Well-Defined Ni/CeO_2 Model Catalyst: Role of Eley-Rideal Reactions.

P. Lozano-Reis, P. Gamallo, R. Sayós, F. Illas

ACS Catal., *14* (2024) 2284-2299.



We report a multiscale study on CO_2 hydrogenation on a Ni/CeO_2 model catalyst combining DFT and kMC simulations. The role of Eley–Rideal steps in water formation is assessed, revealing their often-overlooked impact on activity and selectivity. DFT on $Ni_4/CeO_2(111)$ shows favorable adsorption and low barriers, indicating high selectivity for CO_2 methanation. kMC simulations reveal synergy between two hollow sites of Ni_4, each favoring different elementary steps. This site-dependent reactivity becomes more evident when Eley–Rideal mechanisms are included. Simulations show CO formation via reverse water–gas shift, and methane via $CO_2 \rightarrow CO \rightarrow HCO \rightarrow CH \rightarrow CH_2 \rightarrow CH_3 \rightarrow CH_4$. The results highlight the importance of including Eley–Rideal steps and support the potential of small Ni clusters on $CeO_2(111)$ for selective CO_2 methanation under mild conditions and CO production at higher temperatures.

Line 2. Nanomaterials for emergent technologies

Enzyme Controlled Transient Phospholipid Vesicles for Regulated Cargo Release

A. Venugopal, S. Ghosh, A. Calò, G. M. Tuveri, G. Battaglia, M. Kumar*.

Angew. Chem. Int. Ed., (2025)

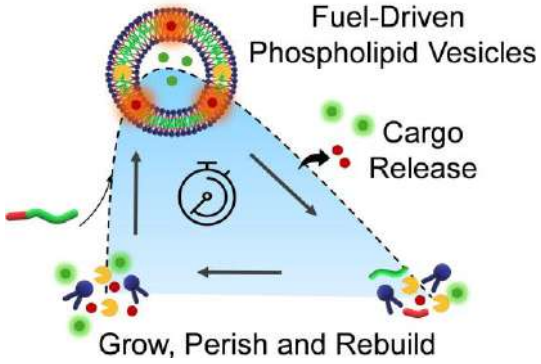


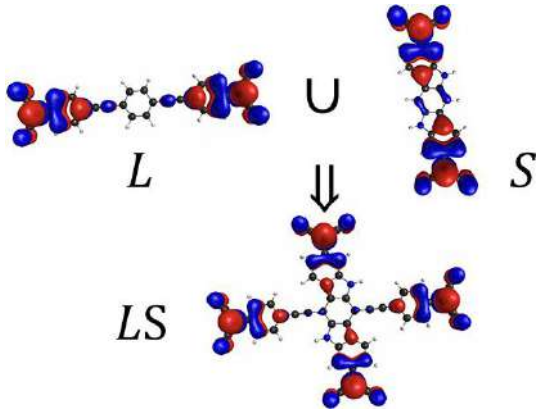
Figure caption: We demonstrate the metabolic formation and degradation of lipids and its chemically fuelled self-assembly into vesicles which can temporally regulate the cargo release.

We describe the in situ formation of a phospholipid and its chemical energy driven assembly into transient vesicles. Our synthetic phospholipid vesicles, which are uniform and 65 nm in diameter, were obtained by a metabolism-like process i.e., formation by simply mixing the precursors and simultaneous degradation by an enzyme. This results in temporally controlled vesicles. Moreover, the cargo release from our vesicles can be dynamically regulated for drug delivery.

Pathway to polyradicals: A planar and fully π-conjugated organic tetraradical(oid).

S. Betkhoshvili, I.d.P.R. Moreira, J. Poater, J.M. Bofill

J. Phys. Chem. Lett., *15* (2024) 5243-5249.

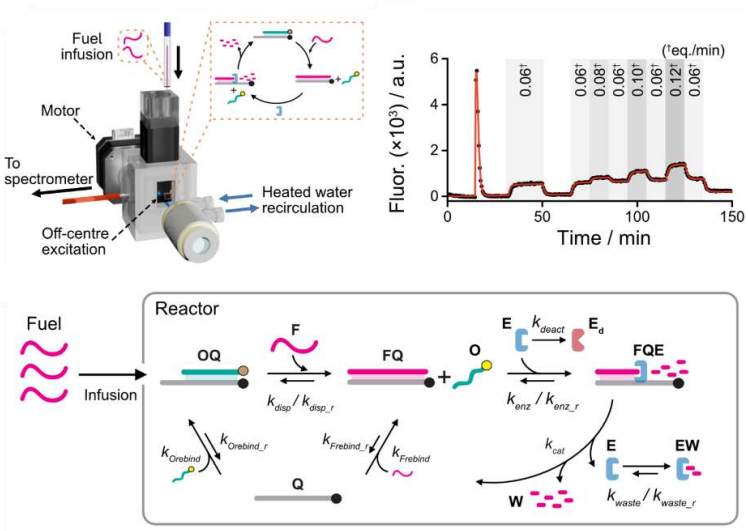


This work presents a strategy to stabilize the ground state of polyradical(oid)s and access higher spin states thermally. As a proof of concept, the authors propose merging two planar, fully π-conjugated diradical(oid)s into a planar, cross-conjugated tetraradical(oid). Multireference quantum chemistry calculations reveal that the resulting molecule is stabilized by π-system aromaticity and delocalization, featuring six thermally accessible spin states within 1.72 kcal/mol. The electronic structure analysis indicates that the π-system comprises two weakly interacting subsystems: aromatic cycles and four unpaired electrons. The stabilization arises from limited conjugation between unpaired electrons, enabled by the aromatic bridging groups, allowing synergistic cross-coupling of the diradical(oid) subunits.

Sustained, reversible and adaptive non-equilibrium steady states of a dissipative DNA-based System

J. D. Nicholas, E. Del Grosso, A. J. De Mello, J. Puigmartí, F. Ricci, A. Sorrenti.

ChemRxiv. 10.26434/chemrxiv-2024-47pw9 (under revision in *Nature Communication*)



In recent years, several chemical fuel-driven supramolecular systems have been reported, aimed at achieving improved kinetic control over self-assembly processes. In parallel, energy-dissipating DNA- based systems have emerged, giving rise to the nascent field of dissipative DNA nanotechnology. Most of these systems rely on batch-wise additions of chemical fuels to closed reactors, which can only generate transient non-equilibrium states. This contrasts with the sustained and highly adaptable non-equilibrium steady states (NESS) achieved by living systems through continuous energy dissipation. In collaboration with the ChemInFlow group, we demonstrate here sustained NESS of a dissipative DNA strand-displacement reaction, achieved through the continuous supply of an RNA fuel to a stirred semi-batch reactor. This was accomplished using a custom automated setup that enables tuneable fuel infusion rates and in situ fluorescence monitoring. Similar to biological NESS, our system dynamically adapts in real-time to subtle variations in fuel supply, approaching different steady-state levels of the strand-displacement reaction on-the-fly. Furthermore, using a kinetic model of the reaction network, we could confirm that the obtained NESS correspond to actual non-equilibrium compositions of the system. This work highlights how moving from closed batch conditions towards thermodynamic openness can enable improved control over dissipative self-assembly processes.

Real-Time Force Monitoring of Electrically Stimulated 3D-Bioengineered Muscle Bioactuators Using Organic Sensors with Tunable Sensitivity

Stefano Lai*, Judith Fuentes, Maria Guix*, Giulia Casula, Piero Cosseddu, Samuel Sánchez*

Advanced Intelligent Systems, (2024) 2400407.

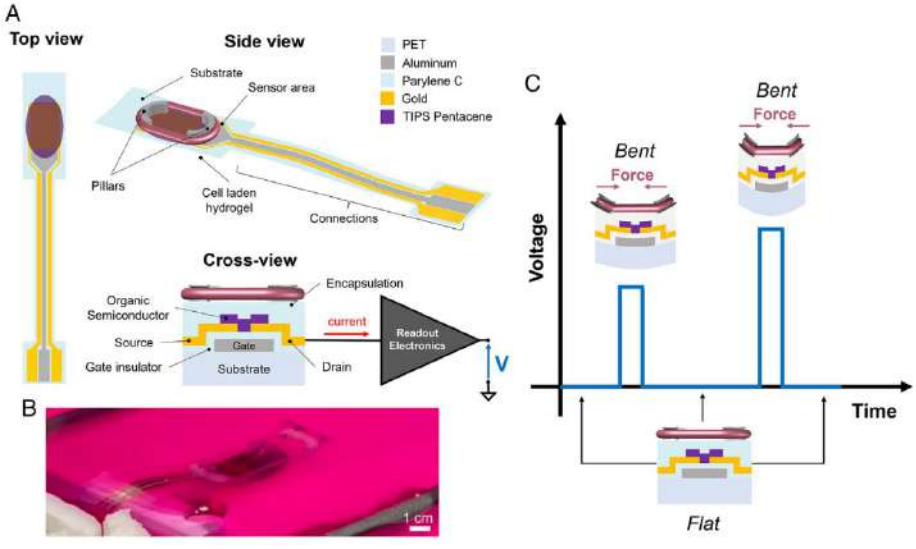


Figure. Schematic of the flexible organic sensor with integrated muscle bioactuator. A) Sensor structure in a top, side, and cross view. Details about structure and materials employed are shown on the latter. B) Picture of the muscle bioactuator assembled in PDMS-based notches on top of the sensor, all set up in a dish with culture media. C) Working principle of the device: when muscle tissue contracts, the sensor is bent, and the output voltage of the readout electronics changes proportionally to the applied strain.

The contractile nature of skeletal muscle tissue makes it especially attractive for powering biohybrid actuators. Significant efforts have been dedicated to the improvement and control of contraction force, going one step forward toward the automation of these biohybrid platforms. Herein, 3D-bioengineered skeletal muscle tissues are integrated with organic transistor-based sensors to define a soft bioactuator with real-time force monitoring capabilities. The muscle tissue is electrically stimulated while the organic sensor ensures transduction of the exerted force into an electrical signal that allows direct monitoring of the bioactuator performance. Sensor calibration is carried out to define its sensitivity at different biasing conditions: as opposed to standard, two-terminal piezoresistive devices, transistor-based strain sensors show tunable sensitivity by acting on the voltage applied to a third terminal—the gate. A complete evaluation of sensing performances is provided, demonstrating that real-time monitoring is effective under different conditions, including stimulation signal frequency and chemical modulation of the bioactuator contraction, demonstrating its potential use as a drug testing platform. In the reported results, the way is paved for a complete exploitation of organic devices in soft robotic applications and to the development of novel biohybrid machines in bioengineering and biomedicine.

Mixed-ligand, radical, gold bis(dithiolene) complexes: from single-component conductors to controllable NIR-II absorbers.

H. Kharraz, P. Alemany, E. Canadell, Y. Le Gal, T. Roisnel, H. Cui, K. H. Kim, M. Fourmigué, D. Lorcy

Chem. Sci., *15* (2024) 11604.

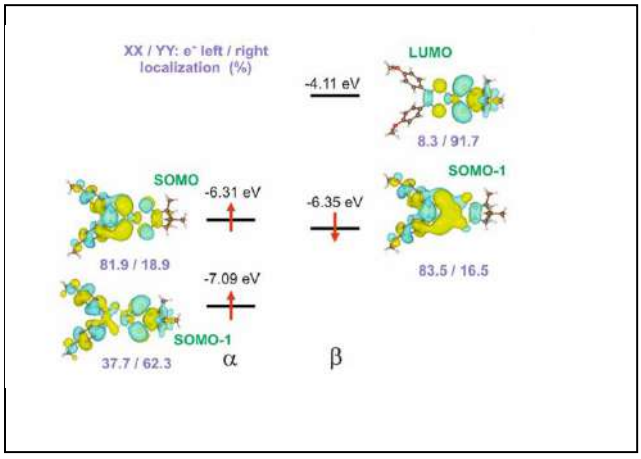


Figure. Frontier orbitals for the asymetric [Au(bdt)(Et-thiazdt)] radical showing the localization on each of the two different ligands.

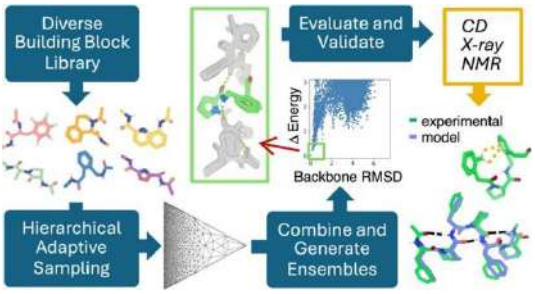
Neutral radical bis(dithiolene) gold complexes [Au(dt)$_2$] absorb strongly in the 1400–2000 nm NIR range. We show that mixed-ligand complexes [Au(dtA)(dtD)] absorb at higher energy, within the desirable NIR-II (1000–1400 nm) range, unlike their symmetric analogs. A selective synthesis of [Au(dtA)(dtD)]$^-$ anions enables the access to unsymmetrical complexes without scrambling. Electrocrystallization yields radical species like [Au(bdt)(Et-thiazdt)] (bdt = benzene-1,2-dithiolate; Et-thiazdt = N-ethyl-thiazoline-2-thione-3,4-dithiolate), which acts as a single-component conductor. Theoretical studies reveal spin polarization, while orbital localization explains their distinct redox and optical properties. The solid-state behavior shows a 1D semiconducting character, stable under pressure up to 18.2 GPa. This method enables a versatile library of mixed-ligand gold complexes with tunable NIR-II absorption and conductor behavior.

Line 3. Biocatalysis and drug discovery

Enumerative Discovery of Noncanonical Polypeptide Secondary Structures

A. P. Moyer, T. A. Ramelot, M. Curti, M. A. Eastman, A. Kang, A. K. Bera, R. Tejero, P. J. Salveson, C. Curutchet, E. Romero, G. T. Montelione and D. Baker.

J. Am. Chem. Soc. *146* (2024) 25501.



Energetically favorable local interactions can overcome the entropic cost of chain ordering and cause otherwise flexible polymers to adopt regularly repeating backbone conformations, like the the α helix present in many proteins. In this article we described a systematic approach to search through dipeptide combinations of 130 chemically diverse unnatural amino acids to identify those predicted to populate unique low-energy states. We characterized ten newly identified dipeptide repeating structures using circular dichroism spectroscopy and simulations, and NMR and X-ray crystallographic structures of two of them were similar to the computational models. Our approach is readily generalizable to identify low-energy repeating structures for a wide variety of polymers, and our ordered dipeptide repeats provide new building blocks for molecular engineering.

Reaction Space Charting as a Tool in Organic Chemistry Research and Development

E. Lozano Baró, P. Nadal Rodríguez, J. Juárez-Jiménez, O. Ghashghaei, R. Lavilla

Adv. Synth & Catal, 366, 4, 551-573, 2024**.**

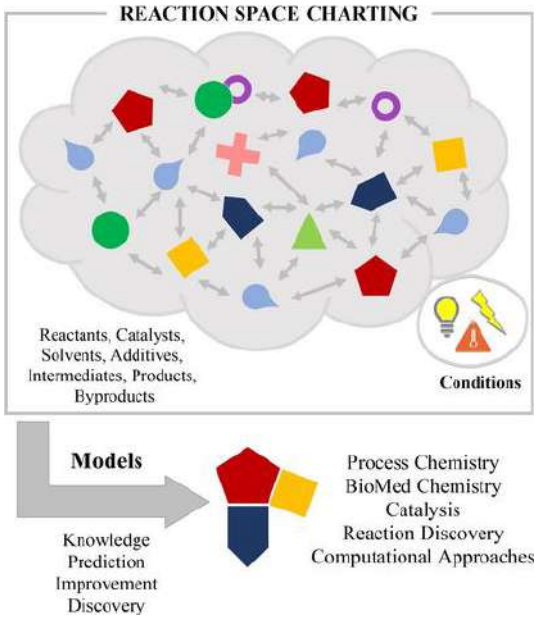


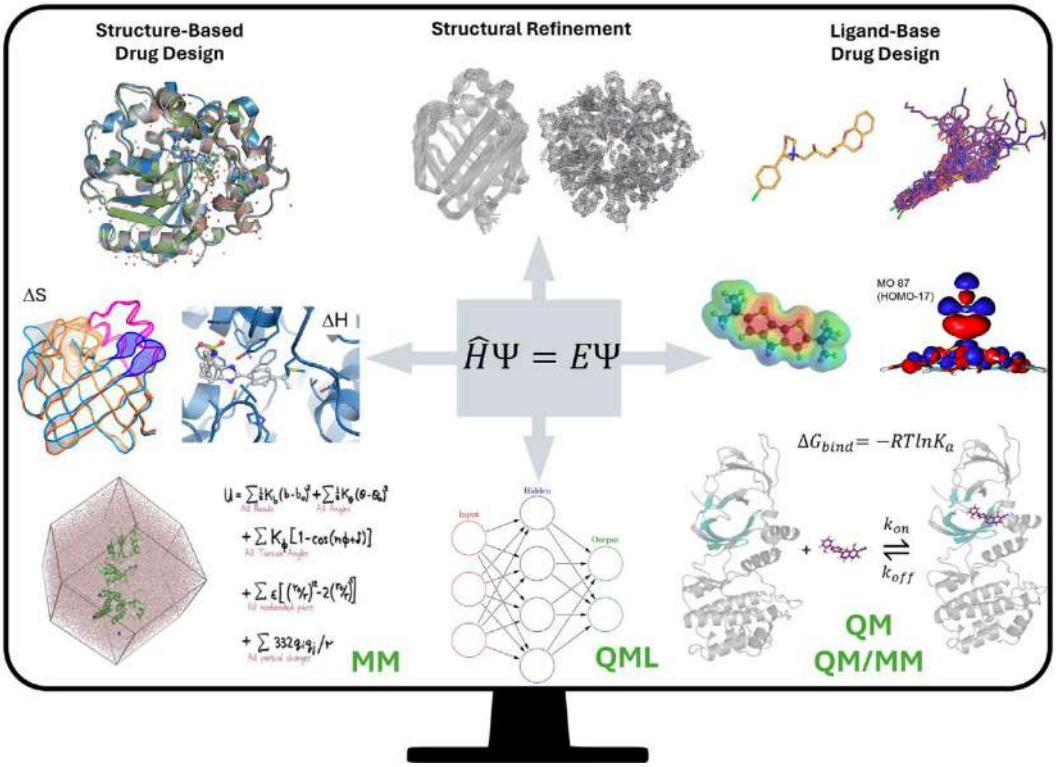
Figure: The concept of reaction space charting

The chemical and reaction spaces are vast, requiring special procedures to study them. Their complex nature involves numerous compounds, interactions, and variable impacts (temperature, solvent, stoichiometry). This necessitates designing, collecting, and analyzing large datasets. Reaction charting, which systematically scans, describes, analyzes, and modifies processes, is a promising approach. It offers fast, accurate solutions and expands system knowledge, enabling reliable predictions and productivity improvements, leading to sustainable, economic, and safe applications. This review introduces the topic, analyzing examples and advancements in organic chemistry. Methodologies range from classical experimentation to Design of Experiments and modern computational approaches like Machine Learning and AI. The impact of charting on process development, biological and medicinal chemistry, catalysis, reaction discovery, and computational methods is discussed. The conclusion provides an appraisal and future prospects for the methodology.

Quantum mechanical-based strategies in drug discovery: Finding the pace to new challenges in drug design

T. Ginex, J. Vazquez, C. Estarellas, F. J. Luque

Curr. Opin. Struct. Biol., *87* (2024) 102870



The expansion of the chemical space to tangible libraries containing billions of synthesizable molecules opens exciting opportunities for drug discovery but also challenges the power of computer-aided drug design to prioritize the best candidates. This directly hits quantum mechanics (QM) methods, which provide chemically accurate properties, but subject to small-sized systems. Preserving accuracy while optimizing the computational cost is at the heart of many efforts to develop high-quality, efficient QM-based strategies, reflected in refined algorithms and computational approaches. The design of QM-tailored physics-based force fields and the coupling of QM with machine learning, in conjunction with the computing performance of supercomputing resources, will enhance the ability to use these methods in drug discovery. The challenge is formidable, but we will undoubtedly see impressive advances that will define a new era.

When can flexible weak polyelectrolytes be treated as effective rigid objects?

J. Orradre, P.M. Blanco, S. Madurga, F. Mas, J.L. Garcés

J. Chem. Phys., *161* (2024) 204906.

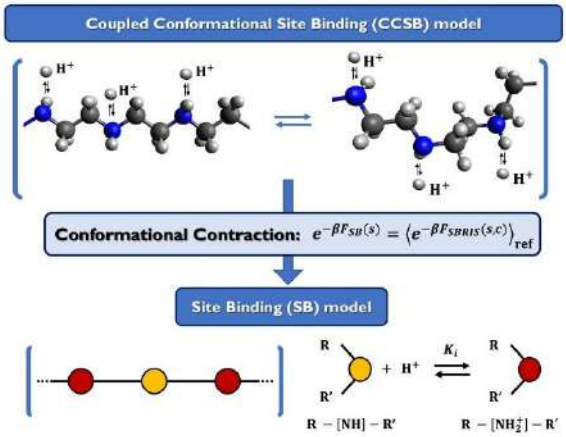


Figure. Averaging procedure over the conformational degrees of freedom using the Conformational Contraction Equations (CCEs). When performing the contraction, an effective rigid object is obtained corresponding to the Site Binding (SB) level of description.

Conformational and ionization equilibria of flexible weak polyelectrolytes (PEs) are, in general, strongly coupled. In this article, we analyze the effect of averaging over (or "contracting") the conformational degrees of freedom so that the original flexible molecule is replaced by an effective rigid object with the same ionization properties. As a result, one obtains the so-called Site Binding (SB) model, much easier to treat both theoretically and computationally, and extensively used to characterize the ionization properties of PE. The conformational averages can be performed in a systematic way by means of the Conformational Contraction Equations (CCEs), which relate the SB parameters to the underlying conformational equilibrium. The conditions for the convergence of the CCE are evaluated in the presence of both Short Range (SR) and Long Range (LR) electrostatic interactions.

Shedding Light on Dark Chemical Matter: The Discovery of a SARS-CoV-2 M^{pro} Main Protease Inhibitor through Intensive Virtual Screening and In Vitro Evaluation

Maria Nuria Peralta-Moreno,Yago Mena,David Ortega-Alarcon,Ana Jimenez-Alesanco, Sonia Vega,Olga Abian,Adrian Velazquez-Campoy,Timothy M. Thomson,Marta Pinto,José M. Granadino-Roldán,Maria Santos Tomas,Juan J. Perez and Jaime Rubio-Martinez

Int. J. Mol. Sci., 25(2024) 6119

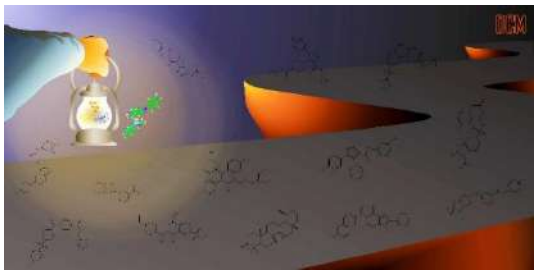


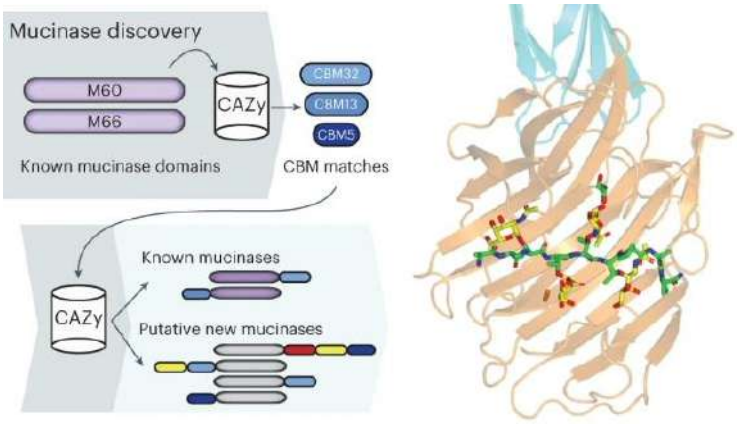
Figura. Shedding Light on Dark Chemical Matter

Dark chemical matter (DCM), a set of drug-like compounds with outstanding selectivity profiles that have never shown bioactivity despite being extensively assayed, appears to be an excellent starting point for drug development. Accordingly, in this study, we performed a high-throughput screening to identify inhibitors of the SARS-CoV-2 main protease (M^{pro}) using DCM compounds as ligands. Multiple receptors and two different docking scoring functions were employed to identify the best molecular docking poses. The selected structures were subjected to extensive conventional and Gaussian accelerated molecular dynamics. From the results, four compounds with the best molecular behavior and binding energy were selected for experimental testing, one of which presented inhibitory activity with a K_i value of 48 ± 5 μM. Through virtual screening, we identified a significant starting point for drug development, shedding new light on DCM compounds.

A family of di-glutamate mucin-degrading enzymes that bridges glycan hydrolases and peptidases

Y. Narimatsu, C. Büll, V. Taleb, Q. Liao, I. Compañón, D. Sánchez-Navarro, F. Durbesson, R. Vincentelli, L. Hansen, F. Corzana, C. Rovira, B. Henrissat, H. Clausen, H. J. Joshi, R. Hurtado-Guerrero

Nat. Catal., *7* (2024) 386-400.



Mucines are sugar covered proteïnes that form a protective barrier in the intestine. Some microbes produce mucinases, enxyms that degrade them. Until now, the majority of known mucinases required metallic ions and only performed on simple sugar chains. A new study by Nature Catalysis descrives a diferent family of mucinases that recognize dense short sugar groupings, especially Tn antígens, tipical of càncer cells. Using modified human mucines, the researchers show that these compounds only act if there are short sugar clústers. The HC7 enzyme stands out for its selectivity and for not using metals, but two glutamates that push a unique two-step mechanism, revealed via computational simulations. When finding similar enzymes and fungus and artròpodes, a wider biological function is suggested with possible aplications in càncer therapy.

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135. H. Ye, C. Franco, M. A. Aboouf, M. Thiersch, S. Sevim, J. Llacer-Wintle, A. Veciana, G. Llauradó-Capdevila, K. Wang, X. Z. Chen, Q. Tang, R. Matheu, P. D. Wendel-Garcia, P. A. Sánchez-Murcia, B. J. Nelson, C. Luo, J. Puigmartí-Luis and S. Pané,"Insights into the Biological Activity and Bio-Interaction Properties of Nanoscale Imine-Based 2D and 3D Covalent Organic Frameworks" *Advanced Science*, **11**.(2024).
136. Y. Yun, D. Lee, S. Lee, S. Pané, J. Puigmartí-Luis, S. Chun and B. Jang,"Enhancing Sensitivity across Scales with Highly Sensitive Hall Effect-Based Auxetic Tactile Sensors" *Advanced Intelligent Systems*, DOI: 10.1002/aisy.202400337.(2024).
137. Y. Zhao, J. Lin, Q. Wu, Y. Ying, J. Puigmartí-Luis, S. Pané and S. Wang,"Revolutionizing Tetracycline Hydrochloride Remediation: 3D Motile Light-Driven MOFs Based Micromotors in Harsh Saline Environments" *Advanced Science*, **11**.(2024).

Book Chapters and Proceedings

Comparative analysis of palladium, nickel and copper phosphane/carbene catalysts in Suzuki–Miyaura couplings: Mechanistic insights and reactivity trends
F. A. Gómez-Mudarra, G. Aullón, J. Jover
Advances in Inorganic Chemistry, *edited by M. Martínez, M. Ferrer and R. Van Eldik* (Elsevier, USA) 2024

Role and impact of glass in chemistry, flow chemistry, and microfluidic technologies
Sevim, S.; Sorrenti, A.; Graniel, O.; Muñoz-Rojas, D.; Pané, S.; Puigmartí-Luis, J.
Additive Manufacturing of Glass: from Science to Applications *edited by Bastian E. Rapp and Frederik Kotz-Helmer* (ELSEVIER, Netherlands) 2024

Greening livestock farming: A multi-platform photo-Biorefinery for sustainable pig slurry management
Prado, A.; Segura, Y.; Pariente, I.; Ventura, M.; Melero, J.A.; Martínez, F.; Serra-Toro, A.; Astals, S.; Mas, F.; Dosta, J.; Puyol, D.

18th IWA. World Conference on Anaerobic Digestion. Conference Proceedings, *edited by ITU Press (Turkey*) 2024

Problem-Based Learning applied to chemistry subjects: face-to-face and online experiences
A. M. Costa; N. Escaja; M. González; S. Madurga; E. Fuguet
Llibre: Active Learning Strategies in Higher Education. Applications in BSc and MSc Degrees of the Faculty of Chemistry at the University of Barcelona , *edited by Nova Science Publishers,* 2024

Other Activities

PHD THESES 2024

Brownmillerite Calcium Ferrite, a Promising Perovskite-Related Material in the Degradation of a Tight Dye under Ambient Conditions
Zahra Noori
Facultat de Química, Universitat de Barcelona & Dhamgan University (Iran)
PhD in Inorganic Chemistry
Jordi Poater, and Azim Malekzadeh
February 2024

Numerical Analysis of Transport Phenomena to Control Reactive Processes in Microfluidic Applications
João Pedro Vale
Porto University
Chemical and Biological Engineering
Dr. Tiago Sotto Mayor and Prof. Josep Puigmartí Luis as a Co-Supervisor
March 2024

Theoretical study of the interplay between structure and spectroscopy in biomolecules
Renato Dias da Cunha
Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona.
PhD Programme in Drug Research, Development and Control
Supervisor Carles E. Curutchet
December 2024

Computational Study on the Application of Two-Dimensional Materials in Hetereogenous Catalysis.
Ling Meng
PhD program: Theoretical Chemistry and Computational Modelling.
Faculty of Chemistry, University of Barcelona.
Supervisors: Francesc Viñes and Francesc Illas
December 2024

Development of materials with increasing structural complexity: from Chiral Stationary Phases to Covalent Organic Polymers and Metal Organic Frameworks
Maria Aurora Guarducci
Sapienza Università di Roma
Pharmaceutical Science
Prof. Claudio Villani and Prof. Josep Puigmartí Luis as a Co-Supervisor
December 2024

Clot-in-a-Chip and Innovative Programmables Materials
Ramón Santiago Herrara Restrepo
Facultat de Química, Universitat de Barcelona.
Nanoscience
Prof. Josep Puigmartí Luis, Prof. Jordi Ignés Mullol
December 2024

Simulations of glycoside hydrolase and phosphorylase reaction mechanism: families GH20, GH29, GH129 and GH130
Irene Cuxart Sánchez
Facultat de Química, Universitat de Barcelona.
Doctoral programme in Organic Chemstry
Carme Rovira
December 2024

Computational modeling of inverting glycosyltransferase reaction mechanisms
Beatriz Piniello Castillo
Facultat de Química, Universitat de Barcelona.
Doctoral programme in Theoretical Chemistry and Computational Modelling
Carme Rovira
December 2024

Master Theses 2024

Sistema de control de procés de producción de ciclohexanol mitjançant una columna reactiva amb un decantador lateral
Andreu Lorente Tribó
Facultat de Química, Universitat de Barcelona.
Master en Enginyeria Química
Dra. Alexandra Elena Plesu Popescu i Dr. Jordi Bonet Ruiz
Febrer 2024

Aplicació del Safety Analyser de Aspen pel disseny i seguretat d'un emmagatzematge de GLP
Joan Ignasi Fernandez Taltavull
Facultat de Química, Universitat de Barcelona.
Master en Enginyeria Química
Dra. Alexandra Elena Plesu Popescu i Dr. Jordi Bonet Ruiz
Febrer 2024

Modelització i simulació d'una biorefineria
Bern Gabarró Alcaraz
Facultat de Química, Universitat de Barcelona.
Master en Enginyeria Química
Dra. Alexandra Elena Plesu Popescu i Dr. Jordi Bonet Ruiz
Febrer 2024

Disseny i Enginyeria del detall d'una columna de destil·lació per la producció de metanol verd
Adam Gabarró Alcaraz
Facultat de Química, Universitat de Barcelona.
Master en Enginyeria Química
Dra Mª Alicia Cardete i Dr. Jordi Bonet Ruiz
Febrer 2024

Estudio de un reactor tubular adiabático de enfriamiento por inyección en frío utilizando un software de dinámica de fluidos computacional (ANSYS)
Florencia Maria Moreyra Schenberger
Facultat de Química, Universitat de Barcelona.
Master en Enginyeria Química
Dra. Alexandra Elena Plesu Popescu i Sr. Ruben Cabello Gallego
Març 2024

Flexible electronics for in situ monitoring of clot-in-chip generation in microfluidic devices
Silvia Veglioni
Master student with a mobility grant from Politecnico di Torino (Italia)
Master's degree in electronic engineering
Prof. Josep Puigmartí Luis and Dr. Maria Guix as a Co-Supervisor
April 2024.

Multi-component supramolecular organic controlled by chemical fuels: building block synthesis and study of self-assembly behaviour
Maria Camacho Molina
Facultat de Química, Universitat de Barcelona.
Master in Organic Chemistry
A. Sorrenti
June 2024.

Transfer learning based on atomic feature extraction for the prediction of experimental ^{13}C chemical shifts.
Žarco Ivković
Facultat de Química, Universitat de Barcelona.
Theoretical Chemistry and Computational Modelling
Supervisor/s: J.Jover, J. N. Harvey
July 2024

Preparation of new Cu(I) MOF structures as catalytic platforms.
Patricia Llanés Lorente
Facultat de Química, Universitat de Barcelona.
Química de Materials Aplicada
Supervisor/s: J.Jover, E. C. Sañudo
July 2024

Estudio computacional de la N-trifluorometilación mediada por cobre de O-benzoilhidroxilaminas.
Rafael Salmerón Vergara
Facultat de Química, Universitat de Barcelona.
Química de Materials Aplicada
Supervisor: J.Jover
July 2024

M090: Mechanisms of binding to Influenza A virus Hemagglutinin.
Maria Rocha
University of Coimbra.
Master in Computational Biology
Pedro Jorge Caridade, F. J. Luque.
July 2024.

CutC reaction mechanism study using QM/MM
Deepti Nehra
University of Barcelona
Erasmus Mundus Master's in Theoretical Chemistry and Computational Modelling
Jeremy Harvey, Carolina Estarellas
July 2024.

Tuning 2D Grazyne Membranes for Biogas Upgrading.
Manel Serrano Rodríguez
MSc. program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
Supervisors: Francesc Viñes and Pablo Gamallo
July 2024.

Optimizing Machine Learning Tools for the Interaction of C on Transition Metal Surfaces.
Gisela Martí Guerrero
MSc. program: Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry.
Faculty of Chemistry, University of Barcelona.
Supervisors: Sergi Vela and Francesc Viñes
July 2024.

Heparin responsive supramolecular nanomaterials for Sensing/diagnostics applications
Fatima Aakki Akhnikh
Facultat de Química, Universitat de Barcelona.
Master in Organic Chemistry
Supervisor/s: Mohit Kumar
July 2024.

Computational analysis of the metabolism and vulnerabilities in colon cancer
Berta Bori-Bru
Facultat de Química, Universitat de Barcelona.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Supervisor/s: Pedro de Atauri, Francesc Mas
July 2024

Integrating Simulations and Experimental Data Treatment: Unveiling the Single-Molecule Mechanical Response of Weak Polyelectrolytes.
Safae El Jelloulil Bota
Facultat de Química, Universitat de Barcelona.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Supervisor/s: Marina Giannotti, Sergio Madurga
July 2024

The influence of mechanical stretching on the conformation and ionization properties of weak polyelectrolyte: linear poly(ethylenimine) as model case.
Marcos Carrera Acosta
Facultat de Química, Universitat de Barcelona.
Master in Atomistic and Multiscale Computational Modelling in Physics, Chemistry and Biochemistry
Supervisor/s: Pablo M. Blanco, Sergio Madurga
July 2024

Activation of Bak protein by molecular fragments
Plazas López, Albert
Facultat de Química, Universitat de Barcelona.
Modelización Computacional Atomística y Multiescala en Física, Química y Bioquímica
Jaime Rubio Martínez
July 2024

Evaluating the use of machine learning to obtain MM-PBSA binding free energies
Roberto Jimenez Villalonga
Facultad de Ciencias. Universidad Autonoma de Madrid.
Master in Theoretical Chemistry and Computational Modelling
Jaime Rubio Martínez
July 2024

Structure determination and computer simulations of the genetically-modified MGAT5 enzyme for biorthogonal chemistry
Laura Meiya Mazo Pirla
Facultat de Química, Universitat de Barcelona.
Erasmus Mundus TCCM Program
Carme Rovira and G.J. Davies
July 2024.

Computational investigation of sugar donor substrate selectivity of N-glycosyltransferases
Pridhi Balhara
Facultat de Química, Universitat de Barcelona. (defense at the University of Groningen)
Erasmus Mundus TCCM Program
Carme Rovira
July 2024.

Synthesis of porphyrin dyads and their application in electron transfer across lipid bilayers.
Arnau Oliveras Tramunt
Facultat de Química, Universitat de Barcelona.
Master in Organic Chemistry
Supervisor: Bart Limburg
July 2024.

Recuperación de nitrógeno amoniacal mediante tecnologías de membrana y modelaje
Tomás Romero Vdal
Facultad de Ciencias, Universidade de Coruña & Facultat de Química, Universitat de Barcelona.
Máster Universitario En Ciencias, Tecnologías Y Gestión Ambiental
Supervisor/s.Alatzne Carlosena, Francesc Mas
September 2024.

Effects of leptin-derived peptides on β-amyloid folding patterns and aggregation inhibition
Mariam Abramishvili
University of Barcelona
Erasmus Mundus Master In Chemical Innovation And Regulation
Carolina Estarellas
September 2024.

Towards the generation of full AMPK model: combining experimental and computational techniques
Adrinê E. Ganimian Tcharkhetian
University of Barcelona
Erasmus Mundus Master In Chemical Innovation And Regulation
Carolina Estarellas
September 2024.

Computational analysis of the conformational space of drug-like compounds.
Roberto D'Onofrio
Università degli Studi di Bari.
Master in Chimica e Tecnologia Farmaceutiche
Cosimo Altomare, F. J. Luque.
November 2024.

ORGANIZATION OF CONGRESSES 2024

Twins in Catalysis: Merging Theory and Experiments
University of Barcelona, Barcelona (Spain)
Organizers: Francesc Viñes, Carme Sousa, Albert Bruix, Ángel Morales.

International Conference on Theoretical of Catalysis (ICTAC 2024)
University of Sevilla, Sevilla (Spain)
International Scientific Board and Chairman: Francesc Viñes
DFT-based kMC simulations of CO_2 hydrogention in Ni_4/CeO_2 catalyst (talk)
P. Lozano-Reis, R. Sayós, F. Illas, P. Gamallo

Active nano/microsystems in the Spanish context (AMES 2024)
Chemistry Faculty, Barcelona (Catalonia, Spain)
Congress Organization: Physics and Chemistry Faculties
Chairman or Organizers: *Dr. Maria Guix Noguera, Dr. Julio Bastos-Arrieta, Prof. Josep Puigmartí Luis, Prof. Ignacio Pagonabarraga*

CECAM School in Kinetics and Dynamics of Chemical Reactions
18-22 March, Zaragoza (Spain)
Congress organization
Chairman or Organizers: Pablo Gamallo, Héctor Prats, Emilio Martínez-Núñez
https://www.cecam.org/workshop-details/school-on-kinetics-and-dynamics-of-chemical-reactions-1343

Scientific conferences and Meetings 2024

Alchemical Free Energy Workshop 2024
BioExcel, Leiden (Netherlands)
14/05/2024
Investigating the allosteric inhibition mechanism of I2 ligands in MAO-B using MD simulations with organic solvent/water mixtures (poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juárez-Jiménez
An unusual His/Asp acid/base dyad in glycosidase catalysis. Insight from QM/MM MD simulations (Poster)
M. Sagiroglugil

13th Congress on Electronic Structure Principles and Applications
Palau de Congressos, Tarragona (Spain)
04/06/2024
Unraveling Cryptophyte Photoacclimation: Insights from Computational Studies on Pigment-Protein Antenna Complexes (talk)
R. D. Cunha, C. Curutchet
Environment effects change FRET distributions in a fluorophore-tagged disordered protein (talk)
D. Gonzalo, C. Curutchet

Meeting of NanoteC24 Carbon Nanoscience and Nanotechnology
Institute of Materials de Nantes Jean Rouxel, Nantes (France)
27/08/2024
The (anti)aromatic properties of cyclo[n]carbons: myth or reality? (oral)
A. J. Stasyuk, G. George, O. A. Stasyuk, M. Solà, F. Plasser

IQTC Meeting 2024
Institut de Química Teòrica i Computacional de la Universitat de Barcelona, Barcelona (Spain)
30/10/2024 - 31/10/2024
Modelling the interplay between structure and spectroscopy in biosystems (talk)
C. Curutchet
Investigating the allosteric inhibition mechanism of I2 ligands in MAO-B using MD simulations with organic solvent/water mixtures (poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juarez-Jiménez
Extending the MST model to large biomolecular systems: parametrization of the ddCOSMO-MST continuum solvation model (poster)
R. D. Cunha, S. Romero, F. Lipparini, F. J. Luque, C. Curutchet
Förster Resonance Energy Transfer Applied to Drug Design (poster)
O. Ergun, M. Castell, X. Barril, C. Galdeano, C. Curutchet
Theoretical mechanistic evaluation of palladium, nickel, and copper catalysts in Suzuki-Miyaura cross-coupling bromides (poster)
F. A. Gómez-Mudarra, G. Aullón, J. Jover
Investigating the allosteric inhibition mechanism of I2 ligands in MAO-B using MD simulations with organic solvent/water mixtures (Poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juárez-Jiménez
From continuum solvation models to the screening of on-demand chemical libraries
F. J. Luque
Exploring the Photoactive Properties of MXenes for Water Splitting (poster)
D. Ontiveros, F. Viñes, C. Sousa
Investigation of the Water Splitting Reaction on ZnO Surfaces in the Excited State (poster)
M. Allés, Á. Morales-García, F. Viñes, M. Nolan
Hydration Accelerates Radiative and Nonradiative Recombination in Small TiO_2 Nanoclusters (poster)

M. Recio-Poo, M. Shakiba, F. Illas, S. T. Bromley, A. V. Akimov, Á. Morales-García
On the CO_2 Harvesting from N_2 Using Grazyne Membranes (poster)
A. Calzada, F. Viñes, P. Gamallo
Understanding the Curvature Effect on Structure and Bonding of MoC_y Nanoparticles on Carbon Supports (poster)
W. Cao, M. Figueras, F. Viñes, F. Illas
The Limits of Ground-State Water Splitting on ZnO surfaces: A Density Functional Theory Study (poster)
R. Morales-Salvador, S.T. Bromley, F. Viñes
Understanding the Formation of Titania/MXene Composites (poster)
M. Keyhanian, N. García-Romeral, Á. Morales-García, F. Viñes, F. Illas
Computational Analysis of Interface Propagation in a Switchable Cooperative $Fe^{(III)}$ Spin-Crossover Material (poster)
D. Ndrio, F. Viñes, A. Gil-Mestres
Growing and Shaping Metal–Organic Framework Single Crystals at the Millimeter Scale' (Poster and speed pitch)
T. Nguyen
The influence of mechanical stretching on the properties of a weak polyelectrolyte (poster)
Carrera, M.; Garcés, J.L.; Mas, F.; Blanco, P.M.; Madurga, S.
Exact Solution for a Freely Joined Chain Polyelectrolyte Model with up to Next Neighbour Interactions (poster)
Orradre, J.; Blanco, P.M.; Madurga, S.; Mas, F.; Garcés, J.L.
Metabolomic and transcriptomic data integration in GSMMs using CORDA (poster))
Bori-Bru, B.; Aleixandre, N.; Pujol-Rigol, S.; López-Blanco, D.; Madurga, S.; Marín, S.; de Atauri, P.; Mas, F.; Cascante, M.

XV Jornada de Recerca de la Facultat de Farmàcia i Ciències de l'Alimentació
Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, Barcelona (Spain)
20/11/2024
Investigating the allosteric inhibition mechanism of I2 ligands in MAO-B using MD simulations with organic solvent/water mixtures (poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juarez-Jiménez
Extending the MST model to large biomolecular systems: parametrization of the ddCOSMO-MST continuum solvation model (poster)
R. D. Cunha, S. Romero, F. Lipparini, F. J. Luque, C. Curutchet
Förster Resonance Energy Transfer Applied to Drug Design (poster)
O. Ergun, M. Castell, X. Barril, C. Galdeano, C. Curutchet

The 27th conference on Process Integration, Modelling and Optimisation for Energy Saving and Pollution Reduction - PRES'24
Xi'an Jiaotong University, Xi'an, (China)
Celebration date (format: 25-28/August/2024)
LNG Cold Energy Recovery for Hydrogen Production Combining Multiple Technologies in Synergy (talk)
C.T. Ferré, R. Cabello, L.M. Marin, A. Plesu, J. Bonet, J. Llorens
Carbon Dioxide to Methanol Valorisation by Process Intensification (talk).
C.T. Ferré, R. Cabello, A.E. Plesu Popescu, J. Bonet-Ruiz, P. Gamallo Belmonte, J. Camps
Discrete Element Method Optimization Simulation of Planetary Ball Mills Operating Conditions (talk)
R. Cabello, J. Han, A.E. Plesu Popescu, J. Bonet-Ruiz, G. Clavé-Batlle, C. Barreneche, S. Dosta
Carbon Dioxide to Methanol Valorisation by Process Intensification (talk).
C. Troyano, R. Cabello, A. E. Plesu, J. Bonet-Ruiz, P. Gamallo, J. Camps

13a Trobada de Joves Investigadors dels Països Catalans
Tarragona (Spain)
29/01/2024
Preparació d'alcohols fluorats: optimització de la síntesi a través de seqüències catalítiques (oral communication)
F. A. Gómez-Mudarra, G. Aullón, J. Jover
Hidrogenació de CO_2 amb Ru encapsulat en silicalita: estudi DFT i model microcinètic (talk)

M. A. Cánovas, R. Sayós, P. Gamallo
Hidrogenció de CO_2 sobre Ni: comparació dels mètodes Monte Carlo cinètic i model microcinètic basats en càlculs DFT (talk)
A. Gracia, P. Lozano-Reis, P. Gamallo, R. Sayós

#RSCPoster Twitter Conference
Virtual
05/03/2024
Assessing Suzuki-Miyaura Cross-Coupling with Nickel Catalyst (poster)
F. A. Gómez-Mudarra, G. Aullón, J. Jover

XX Reunión Bienal del Grupo Especializado de Química Inorgánica y XIV Reunión Bienal del Grupo Especializado de Química del Estado Sólido de RSEQ
La Coruña (Spain)
04/06/2024
Exploring the landscape in copper(I)-catalyzed oxidative addition of aryl and alkyl bromides (oral communication)
F. A. Gómez-Mudarra, G. Aullón, J. Jover

Electronic Structure Principles and Applications and biennial Meeting of the RSEQ Group in Chemistry and Computation
Tarragona (Spain)
06/06/2024
Exploring the landscape in copper(I)-catalyzed oxidative addition of aryl and alkyl bromides (oral communication)
F. A. Gómez-Mudarra, G. Aullón, J. Jover

AI for Accelerated Materials Design - Vienna 2024
Vienna (Austria)
27/07/2024
Transfer learning based on atomic feature extraction for the prediction of experimental ^{13}C chemical shifts (oral communication)
Ž. Ivković, J. Jover, J. N. Harvey

European Colloquium on Inorganic Reaction Mechanisms 2024
Toulouse (France)
09/09/2024
Exploring the landscape in copper(I)-catalyzed oxidative addition of aryl and alkyl bromides (oral communication)
F. A. Gómez-Mudarra, G. Aullón, J. Jover
Catalytic Synthesis of Fluorinated Alcohols from Alkenes and Ketones (oral communication)
F. A. Gómez-Mudarra, J. Jover, G. Aullón

#LatinXChem24 Conference
Virtual
14/10/2024
Theoretical mechanistic evaluation of palladium, nickel, and copper catalysts in Suzuki-Miyaura cross-coupling bromides (poster)
F. A. Gómez-Mudarra, G. Aullón, J. Jover

Twins in Catalysis: Merging Theory and Experiment
Barcelona (Spain)
21/11/2024
Theoretical mechanistic evaluation of palladium, nickel, and copper catalysts in Suzuki-Miyaura cross-coupling bromides (poster)
F. A. Gómez-Mudarra, G. Aullón, J. Jover

Exploring the Photoactive Properties of MXenes for Water Splitting (poster)
D. Ontiveros, F. Viñes, C. Sousa
Understanding the Formation of Titania/MXene Composites (poster)
N. García-Romeral, M. Keyhanian, Á. Morales-García, F. Viñes, F. Illas
A Computational Map of the Probe CO Molecule Adsorption and Dissociation on Transition Metal Low Miller Indices Surface (poster)
D. Vázquez-Parga, A. Jurado, A. Roldán, F. Viñes
Assessing Adsorbate-Solvent Interaction and the Role of Dispersive Forces (poster)
E. Romeo, F. Illas, F. Calle-Vallejo
Atomic Hydrogen Interaction with Transition Metal Surfaces: A High-Throughput Computational Study (poster)
M. Allés, L. Meng, I. Beltrán, F. Fernández, F. Viñes
Understanding the Reverse Water Gas Shift Reaction over Mo_2C MXene Catalyst: A Holistic Computational Analysis (poster)
D. Dolz, R. De Armas, P, Lozano-Reis, Á. Morales-García, F. Viñes, R. Sayós, F. Illas
Hydration Accelerates Radiative and Nonradiative Recombination in Small TiO_2 Nanoclusters (poster)
M. Recio-Poo, M. Shakiba, F. Illas, S. T. Bromley, A. V. Akimov, Á. Morales-García
On the CO_2 Harvesting from N_2 Using Grazyne Membranes (poster)
A.Calzada, F. Viñes, P. Gamallo
Understanding the Curvature Effect on Structure and Bonding of MoCy Nanoparticles on Carbon Supports (poster)
W. Cao, M. Figueras, F. Viñes, F. Illas
Surface Termination Modulated Catalytic Activity of Ti_3C_2 MXene HER and CO_2RR (poster)
L. Meng, F. Viñes, F. Illas
Environment Factors in Computational Catalysis (plenary lecture)
F. Viñes
From CO on MgO to catalytic nanomaterials (invited talk)
K.M. Neyman
CO_2 conversion using H_2 on silicalite-encapsulated Ru atoms: a DFT and Microkinetic modeling study (poster)
M. Cánovas, R. Sayós, P. Gamallo
DFT study of Methane dehydrogenation on the $Ni_2Cu_2@Al_2O_3$ catalyst Surface (poster)
S. Benchikh, M. F. Haroun, K. Kassali, P. Gamallo
Microkinetic Modeling vs kinetic Monte Carlo Simulations: choosing the right kinetic approach to unravel the CO_2 hydrogenation (poster)
A. Gracia, R. Sayós, P. Gamallo
On the CO_2 Harvesting from N_2 using Grazyne Membranes (poster)
A. Calzada, F. Viñes, P. Gamallo

IPR Training for Researchers & ESR Presentations on the Progress of their Research
Belgium
27/02/2024
Allosteric ligands of FBXW7 E3 ligase (Presentation)
V. Ivanova, J. Juárez-Jiménez

11th International BSC Severo Ochoa Doctoral Symposium 2024
Barcelona, Spain
07/05/2024
Development of novel non-peptidic VHL binders using a fragment-based approach (Talk)
P. Blanco-Gabella, K. Haubrich, R. Casement, V. Spiteri, C. Galdeano, J. Juárez-Jiménez, A. Ciulli, X. Barril

Alchemistry Workshop on Free Energy Methods in Drug Design
Netherlands
13/05/2024
Investigating the allosteric inhibition mechanism of I2 ligands in MAO-B using MD simulations with organic solvent/water mixtures (Poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, J. Juárez-Jiménez, C. Curutchet

Alchemistry Workshop
Netherlands
13/05/2024
Understanding cooperativity effects in the drug-dependent degradation of the Cereblon neosubstrate CK1 (Poster)
M. Miñarro-Lleonar, A. Bertran-Mostazo, J. Duro, X. Barril, J. Juárez-Jiménez
OpenDuck: a python library for steered MD (Poster)
Á. Serrano-Morrás, S. Bray, J. Juárez-Jiménez, X. Barril

Protein Degradation in Focus 2024 Symposium
Dundee, United Kingdom
19/05/2024
Development of novel non-peptidic VHL binders using a fragment-based approach (Poster)
P. Blanco-Gabella, K. Haubrich, R. Casement, V. Spiteri, C. Galdeano, J. Juárez-Jiménez, A. Ciulli, X. Barril

ALLODD 3rd Training School & Networking Meeting
Urbino, Italy
10/06/2024
Towards a mechanistic understanding of Molecular Glues: Insights from the CRBN-Lenalidomide-CK1α complex (Invited Talk)
J. Juárez-Jiménez
Allosteric ligands of FBXW7 E3 ligase (Presentation)
V. Ivanova, J. Juárez-Jiménez

Bioexcel Summer School on Biomolecular Simulations 2024
Pula, Italy
16/06/2024
Molecular Glues in Drug Design: Enhancing Protein-Protein Interaction Stability for Innovative Cancer Therapies (Poster)
B. Díaz-Canals, J. Juárez-Jiménez

The 10th Annual CCPBioSim & MGMS 2024 Conference: Molecular Modelling in Structure-Based Drug Design
England
01/07/2024
Computational binding mode elucidation of Fbw7 E3 ligase fragment hits through Multiple-copies Association Studies (MAS) (Poster)
V. Ivanova, R. Castaño, C. Galdeano, J. Juárez-Jiménez, X. Barril
Development of novel non-peptidic VHL binders using a fragment-based approach (Poster)
P. Blanco-Gabella, K. Haubrich, R. Casement, V. Spiteri, C. Galdeano, J. Juárez-Jiménez, A. Ciulli, X. Barril

X SEQT Young Researchers Symposium
Madrid, Spain
12/07/2024
Development of novel non-peptidic VHL binders using a fragment-based approach (Poster)
P. Blanco-Gabella, K. Haubrich, R. Casement, V. Spiteri, C. Galdeano, J. Juárez-Jiménez, A. Ciulli, X. Barril

XXVIII EFMC International Symposium on Medicinal Chemistry
Italy
01/09/2024
Multiple-copies association studies (MAS) for computational binding mode elucidation of Fbw7 E3 ligase fragment hits (Poster)
V. Ivanova, R. Castaño, C. Galdeano, J. Juárez-Jiménez, X. Barril

11th EFMC Young Medicinal Chemists' Symposium
Italy
05/09/2024
Multiple-copies association studies (MAS) for computational binding mode elucidation of Fbw7 E3 ligase fragment hits (Poster)
V. Ivanova, R. Castaño, C. Galdeano, J. Juárez-Jiménez, X. Barril

24th European Symposium on Quantitative Structure-Activity Relationship (EuroQSAR)
Barcelona, Spain
22/09/2024
Molecular Glues in Drug Design: Enhancing Protein-Protein Interaction Stability for Innovative Cancer Therapies (Poster)
B. Díaz-Canals, J. Juárez-Jiménez
Computational binding mode elucidation of FBW7 E3 ligase fragment hits through multiple-copies association studies (MAS) (Presentation)
V. Ivanova, R. Castaño, C. Galdeano, J. Juárez-Jiménez, X. Barril
Towards a mechanistic understanding of molecular glues: insights from the CRBN-Lenalidomide-CK1α complex (Poster)
M. Miñarro-Lleonar, A. Bertrán-Mostazo, J. Duro, X. Barril, J. Juárez-Jiménez
Developing a movel scoring function empowered by QM-derived hydrophobicity descriptors
B. Medel-Lacruz, W. J. Zamora, E. Herrero, G. E. Kellogg, J. Vázquez, F. J. Luque
Exploring SARS-Cov-2 main protease binding site with PharmQSARB. Medel-Lacruz, W. J. Llop-Peiró, A.; Luque, F. J.; Ginex, T.; Garcia-Vallvé, S.; Pujadas, G.
Computational tools for understanding disorder to order transitions upon ligand binding
S. Llabrés, C. Mendoza-Martínez, M. Papadourakis, J. Michel
Exploring the opportunities of machine learning for binding energy prediction
R. Jiménez-Villalonga; MN. Peralta-Moreno, M. Shevelev, M.Cascante, J. Rubio-Martínez
Exploring the limits of fragment dissolved molecular dynamics
MN. Peralta-Moreno, J. Rubio-Martínez, JM. Granadino-Roldán
Disrupting SARS-CoV-2'S Inflammasome activation with smal-molecula inhibitors targeting Orf9b
N. DeMoya Valenzuela, E. Zodda, M. Pons, C. Calvo-González,C. Benítez-Rodríguez, BD. López-Ayllón, A. Hibot, M. Cascante, M. Montoya, MD. Pujol, J. Rubio-Martínez, TM. Thomson
A Robust virtual screening protocol for drug discovery
JM. Granadino-Roldán, MN. Peralta-Moreno, N. DeMoya-Valenzuela, J. Rubio-Martínez

XV Jornada de Recerca de la Facultat de Farmàcia i Ciències de l'Alimentació
Barcelona, Spain
20/11/2024
Investigating the allosteric inhibition mechanism of I2 ligands in MAO-B using MD simulations with organic solvent/water mixtures (Poster)
B. Ozaydin, C. Griñán-Ferré, A. Bagán, M. Pallàs, C. Escolano, C. Curutchet, J. Juárez-Jiménez

2a Reunió de Química Teòrica i Computacional (RQTC)
Barcelona, Spain
30/01/2025
Adhesius moleculars en el disseny de fàrmacs: millorant l'estabilitat de les interaccions proteïna-proteïna per a teràpies contra el càncer (Poster)
B. Díaz-Canals, J. Juárez-Jiménez

Evotec
Toulouse, France
30/05/2024
Conformational analysis of drug-like molecules: Challenges in the search of the bioactive conformation
F. J. Luque
Continuum solvation models of solvation and hydrophobicity
F. J. Luque

Nostrum Biodiscovery
Barcelona, Spain
14/06/2024
Facing the challenges of the explosive expansion of the chemical space
F. J. Luque

4th Molecules Medicinal Chemistry Symposium — Harnessing the Power of New Drug Modalities
Barcelona, Spain
24/04/2024
VF-57: Targeting the release of the fusion peptide in Influenza A virus hemagglutinine
A. Valdivia, V. Francesconi, V.; C. Escriche, S. Vázquez, S. Rimaux, L. Naessens, F. J Luque

European Workshop in Drug Design 2024
Siena, Italy
19/05/2024
Application of quantum mechanical 3D atomic models of hydrophobicity in virtual screening and drug design
F. J Luque

7th Innovative Approaches for Identification of Antiviral Agents Summer School
Santa Margherita di Pulia, Italia
23/09/2024
Novel fusion inhibitors targeting hemagglutinin (HA) of influenza A H1N1 virus
A. De la Cruz, S. Velázquez, L. Naesens F. J. Luque, M. J. Camarasa, S. De Castro, S.

Nextflow Summit 2024 | Barcelona
World Trade Center, Barcelona (ES)
28/10/2024 - 03/11/2024
Automatization of the Bottom-up Exploration of the Chemical Space for the Early Drug Discovery
S. Llabrés, Á. Serrano-Morrás, C. Galdeano, J, Juárez-Jiménez, Xavier Barril

X Symposium of Medicinal Chemistry Young Researchers
Madrid, Spain
12/07/2024
Effects Of Leptin-Derived Peptides On B-Amyloid Folding Patterns and Aggregation Inhibition
M. Abramishvili, C. Estarellas

VI QuimBioQuim - Congreso de Jóvenes Químicos y Bioquímicos Terapéuticos
Jaén, Spain
25/10/2024
Assessing the molecular factors involved in the inhibition of Choline Trimethylamine-Lyase
M. Gómez, C. Estarellas

IV Congreso internacional CyTA Junior
Barcelona, Spain
02/04/2024
Exploring molecular factors of specific CUTC/CUTD enzymes from gut microbiome: The Importance of choline metabolism in the regulation of CVDs
A. Palomares Moyano, C. Estarellas

XXVIII EFMC International Symposium on Medicinal Chemistry (EFMC-ISMC 2024)
Rome, Italy
01/09/2024
Unveiling The Key Role of Allosteric Adam Activators On The Isoform selectivity of AMPK
K. Barmpidi; R. Evans; F. J. Luque; C. Estarellas
Novel strategy against tuberculosis disease: Understanding the essentiality of Ndh
K. Barmpidi, C. Estarellas, F. J. Luque

International Workshop on Multiscale Computational Design for Heterogeneous Functional Materials
Federico II Congress Center, Naples (Italy)
14–15/2/2024
Effect of Water on Photoactive TiO_2 Nanostructures: Implications in Heterogeneous Photocatalysis (invited talk)
Á. Morales-García

DPG Spring Meeting 2024
Technical University of Berlin, Berlin (Germany)
17–22/3/2024
MXenes as Materials for Carbon Capture, Storage, and Usage Technologies: Computational Insights & Predictions (invited talk)
F. Viñes

Graphene2024 Conference
Space Pablo VI, Madrid (Spain)
25–28/6/2024
Grazynes: New 2D Materials for Biogas Upgrading (poster)
A. Calzada, F. Viñes, P. Gamallo
Properties and Applications of Grazynes: Carbon-Based 2D Composites (talk)
P. Gamallo, A. Calzada, F. Viñes
New Membranes for Biogas Upgrading? (poster)
A. Calzada, F. Viñes, P. Gamallo

EUROMXENE Congress
Polytechnical University of Valencia, Valencia (Spain)
26–28/6/2024
Computational Study of MXenes for Water Splitting Photocatalysis (flash talk and poster)
D. Ontiveros, F. Viñes, C. Sousa
Understanding MXenes from First Principles (plenary lecture)
F. Illas

Insights on the Nature of the Chemical Bond of Composites Made of TiO_2 Clusters Supported on Ti_2C from Density Functional Theory (flash talk and poster)
N. García-Romeral, M. Keyhanian, Á. Morales-García, F. Viñes, F. Illas
Surface Termination Modulated Catalytic Activity of Ti_3C_2 MXene HER and CO_2RR (flash talk and poster)
L. Meng, F. Viñes, F. Illas

Electronic Structure: Principles and Applications (ESPA2024)
Congress and Fair Palace of Tarragona, Tarragona (Spain)
3–7/7/2024
Understanding The Magnetic Nature of Bare MXenes in their Electronic Ground State (poster)
N. García-Romeral, Á. Morales-García, F. Viñes, I.d.P.R. Moreira, F. Illas
Tuning Electronic Levels in Photoactive Hydroxylated Titania Nanosystems: Combining the Ligand Dipole Effect and Quantum Confinement (talk)
M. Recio-Poo, Á. Morales-García, F. Illas, S. T. Bromley
Towards Polyradicals: A Planar and Fully π-Cojugated Organic Tetraradical(oid) (poster)
J. M. Bofill

QM/MM studies of protein glycosylation reactions (Oral communication)

C. Rovira
An unusual His/Asp acid/base dyad in glycosidase catalysis. Insight from QM/MM MD simulations (Oral communication)
M. Sagiroglugil
Molecular mechanism and determinants for the unique specificity of the Akkermansia muciniphila sialidase GH181 (Oral communication)
M. Corbella
Multiscale approach for CO_2 hydrogenation on Silicalite-encapsulated Ru atoms (poster)
M. Cánovas, R. Sayós, P. Gamallo
A comparative kinetic study of the CO_2 hydrogention on Ni(111) surface: microkinetic modeling vs. kinetic Monte Carlo simulations (poster)
A. Gracia, P. Lozano-Reis, P. Gamallo, F. Huarte, R. Sayós
Solvation effects in the reaction profiles of the hydrogenation of Nitrobenzene to Aniline catalyzed on Palladium (comunicació oral)
J. Herrera, G. Alonso, P. Gamallo

18th International Congress on Catalysis (ICC 2024)
Lyon Convention Centre, Lyon (France)
14–19/7/2024
Comprehensive Analysis of Excited States in Photoactive Titania Nanostructures (poster)
Á. Morales-García, M. Recio-Poo, S. T. Bromley, F. Illas
Computational Assessment of MXenes Bandgap Engineering for the Photocatalytic Water Splitting (talk)
D. Ontiveros, S. Vela, C. Sousa, F. Viñes
Quantifying elusive interface effects in catalytic nanomaterials combining DFT modelling and experiment (talk)
K.M. Neyman

XV International Congress in Chemical Teaching and Research
Metropolitan Autonomous University of Azcapotzalco, Mexico DF (Mexico)
24–26/7/2024
Computational Design of Realistic TiO_2 Nanostructures with Heterogeneous Photocatalysis Implications (invited talk)
Á. Morales-García

International Conference on Theoretical Aspects of Catalysis (ICTAC 2024)
University of Sevilla, Sevilla (Spain)
2–6/9/2024

Analyzing Activity and Selectivity Trends for NO Hydrogenation Using "Catalytic Matrices" (talk)
E. Romeo, F. Illas, F. Calle-Vallejo
Investigation of the Water Splitting Reaction on ZnO Surfaces in the Excited State (poster)
M. Allés, Á. Morales-García, F. Viñes, M. Nolan
Investigating the Excited State Properties of Photoactive Hydrated TiO_2 Nanoclusters Through Non-Adiabatic Molecular Dynamics (poster)
M. Recio-Poo, M. Shakiba, F. Illas, S. T. Bromley, A. V. Akimov, Á. Morales-García
Influence of Water in the Structure and the Band Edges of Photoactive Titania Nanoparticles: Implications in Photocatalysis (invited talk)
Á. Morales-García

XXIX CICAT Ibero-American Catalysis Congress – Bilbao 2024
Euskalduna Conference Centre, Bilbao (Spain)
23–27/9/2024
Transition Metal Carbides of V, Nb and Ta for CO_2 Capture and Activation (talk)
H. Prats, A. Pajares, F. Viñes, P. Ramírez de la Piscina, R. Sayós, F. Illas, N. Homs

FOTOFUEL School
IMDEA Energy Institute, Madrid (Spain)
15–16/11/2024
Hydrated Small TiO_2 Nanoclusters: Implications in the Nonradiative Recombination (invited talk)
Á. Morales-García

Computational Modeling of Catalysis: Challenges and Opportunities
University of Évora, Évora (Portugal)
27/11/2024
MXenes for CO_2 Capture, Storage, and Conversion Technologies (invited talk)
F. Viñes

Active nano/microsystems in the Spanish context
University of Barcelona, Barcelona,
24-25/10/2024
Chemically fueled active vesicles for temporally controlled cargo release (invited talk)
M. Kumar
From Dust to Design with Microfluidic Tools' (talk)
J. Puigmartí-Luis (member of the congress organizers. Invited by Dr. Maria Guix and Dr. Julio Bastos)
Growing and Shaping Metal–Organic Framework Single Crystals at the Millimeter Scale' (Poster)
T. Nguyen

ESAB 2024-European South Atlantic Biophysics Congress
San Sebastian, Spain,
5-7/06/2024
Vesicles: Nanocontainers for temporally regulated cargo delivery (invited talk).
M. Kumar

IBEC – KAIST Symposium
IBEC, Barcelona,
20/05/2024
Active Vesicles for temporally regulated cargo delivery (**Invited symposium talk)**
M. Kumar

Indian Institute of Technology, Bombay (Mumbai-India)
05/01/2024
Active Vesicles: Nanocontainers for temporally regulated cargo delivery (**Invited department seminar**)
M. Kumar

International Workshop on Macromolecular Materials
San Sebastián (Spain)
11/06/2024
Boron Extension Drives to the Facile Construction of New Hybrid Conjugated Materials (talk)
J. Poater

III Simposio Jóvenes Investigadores RANME
Madrid (Spain)
04/07/2024
Cooperatividad en macrociclos derivados de bases de ADN unidos por enlaces por puente de hidrogeno (invited talk)
J. Poater

5th Workshop on Magnetically Induced Molecular Currents (MAGIC) 2024.
Frauenwörth (Germany)
9/09/2024.
Facile Construction of New Hybrid Conjugation via Boron Cage Extension (invited talk)
J. Poater

4th European Symposium on Chemical Bonding (CBOND2024)
Amsterdam (The Netherlands)
24/09/2024
On the existence of collective interactions reinforcing the metal-ligand bond in organometallic compounds *(invited talk)*
J. Poater

4th International Conference on Carbon Chemistry and Materials
Barcelona (Spain)
11/11/2024
Fusion of Polycyclic Aromatic Hydrocarbons to Boron Clusters (invited talk)
J. Poater

12th International Chemistry Conference
Singapore (Singapore)
9/12/2024
Boron Cage Extension: from Cluster-Phosphonim Conjugates to Cluster-Cored Trycyclics with Alkynes (invited talk)
J. Poater

MES2024 7th International Conference on Molecular Electronic Structure
Pescara (Italy)
7/6/2024
Towards Polyradicals: A Planar and Fully π-Cojugated Organic Tetraradical(oid) (poster)
J. M. Bofill

Workshop "Bio-hybrids: When robots get alive", organized in the framework of the Robosoft 2024 (7 th IEEE-RAS International Conference on Soft Robotics)

14/04/2024 (San Diego, USA)
'Modulating Control And Functionality in Skeletal Muscle Robots' (talk)
M. Guix (invited by Prof. Miriam Filippi as a Workshop invited speaker)

12th World Biomaterials Congress (WBC 2024)
26 – 31/05/2024) Daegu, Corea
'Revolutionizing Materials Engineering and Processing with Microfluidic Tools' (talk)
J. Puigmartí-Luis (invited by Prof. Jae-Byum Chang as a Symposium invited speaker)

AIM24 — Artificial Intelligence for iMaging 2024
26/05-01/06/2024 Sant Carles de la Ràpita, Spain
'Exploring the Intersection of AI in Designing and Controlling Living Robots' (talk)
M. Guix (invited by Prof. Carlo Manzo)

Nanomotors conference Barcelona
3– 5/06/2024 Barcelona, Catalonia, Spain
'*Revolutionizing Materials Engineering and Processing with Microfluidic Tools' (talk)*
J. Puigmartí-Luis (invited by Prof. Samuel Sanchez Ordóñez)
'*Tailoring functionality and control in living robots across scales' (talk)*
M. Guix (invited by Prof. Samuel Sanchez Ordóñez)

3rd Annual Nanoseries Conference
17 – 19/06/2024 Lisboa, Portugal
'*Revolutionizing Materials Engineering and Processing with Microfluidic Tools' (talk)*
J. Puigmartí-Luis (invited by Prof. Jose Paulo Farinha)

N.I.C.E. Conference
19 – 21/06/2024 Nice, France
'*Revolutionizing Materials Engineering and Processing with Microfluidic Tools' (talk)*
J. Puigmartí-Luis (invited by Prof. Frédéric Guittard as a Keynote speaker)

International Conference on Manipulation, Automation and Robotics at Small Scale (MARSS2024)
1 – 5/07/2024 Delf, Netherlands
'Revolutionizing Materials Engineering and Processing with Microfluidic Tools' (talk)
J. Puigmartí-Luis (invited as a Plenary speaker)
Title: *'Moving living robots to the microscale' (talk)*
M. Guix (invited by Prof. Loai Abdelmohsen in the Nano and micromotors: Motion fundamentals and applications Special Session)

CMD – General Conference of the Condensed Matter
2-6/09/2024 Braga, Portugal
'*Design and performance of soft biohybrid swimmers' (talk)*
M. Guix (invited by Prof. Rodrigo Coelho)

9th International Conference on Metal-Organic Frameworks and Open Framework Compounds (MOF2024)
15 – 19/09/2024 Singapore, Republic of Singapore
'*Revolutionizing Materials Engineering and Processing with Microfluidic Tools' (talk)*
J. Puigmartí-Luis (invited by Prof. Dan Zhao)
'*Tailored design of a water-based nanoreactor technology for producing processable sub-40 nm 3D COF nanoparticles at atmospheric conditions' (talk)*
G. Llauradó-Capdevila
'Growing and Shaping Metal–Organic Framework Single Crystals at the Millimetre Scale' (Poster)
T. Nguyen

Twilight Conference
21-22/09/2024 Madrid, Spain
'Improving Biohybrid Muscles for Smarter, Stronger Soft Robots*' (talk)*
M. Guix

European Research Night: Bringing researchers into the light. (101162311/HORIZON-MSCA- 2023-CITIZENS-01 (Marie Sklodowska-Curie-European Night of Researchers and actions of Researchers in Schools 2024 - 2025))
27/09/2024 València, Spain
'Microrobotics, biomedicine and videogame controllers*' (talk)*
M. Palacios
'Robots vius a la carta*' (talk)*
M. Guix

Fall meeting & Exhibit (2024 MARS)
01 – 06/12/2024 Boston, Massachusetts
Title: *'Microfluidic tools for the bioinspired synthesis of artificial functional materials' (talk)*
J. Puigmartí-Luis

N.I.C.E. Winter Event
10 – 12/12/2024 Nice, France
'Microfluidic Tools for the Bioinspired Synthesis of Artificial Functional Materials' (talk)
J. Puigmartí-Luis (Invited by Frédéric Guittard)

Masterquímica XIX
Venue, Barcelona (Spain)
Celebration date (21-22/5/2024)
Identificació de dianes terapèutiques en el metabolisme tumoral mitjançant models computacionals (poster)
Bori-Bru, B.; López-Blanco, D., Martín, S.; Madurga, S.; Cascante, M. de Atauri, P.; Mas, F.
La influència de l'estirament mecànic en les propietats d'un polielectròlit feble
Carrera, M.; Garcés, J.L.; Mas, F.; Madurga, S.; Blanco, P.M.

II SESMET Conference
Venue, Sevilla (Spain)
Celebration date (3/6/2024)
Multi-omics data integration into Genome-Scale Metabolic Models reveals distinctive metabolic vulnerabilities associated to FOLFOX chemotherapy resistance in colorectal cancer (talk)
Cascante, M.; Perez-León, R.; López-Blanco, D.; Bori-Bru, B.; Madurga, S.; Tarrado-Castellarnau, M.; Mas, F.; de Atauri P.; Marin S.
Distintive metabolic colorectal cancer subtypes identifyed by multi-omics data integration (poster)
Marin, S.; López-Blanco, D.; Foguet, C.; Tarrado-Castellarnau, M.; Centelles, JJ.; Madurga, S.; Cascante, M.

18th IWA World Conference on Anaerobic Digestion
Venue, Istanbul (Turkey)
Celebration date (4/6/2024)
Greening livestock farming: A multi-platform photobiorefinery for sustainable pig slurry management (talk)
De Nicolás, A.P., Ventura, M.; Segura, Y.; Pariente, I.; Melero, J.A.; Martínez, F.; Serra-Toro, A.; Astals, S.; Mas, F.; Dosta, J.; Puyol, D.

Molecular Modelling of Charged (Bio)Macromolecules Systems Workshop
Venue, Trondheim (Norway)
Celebration date (17/6/2024)
When can Flexible Weak Polyelectrolytes be tretated as Effective Rigid Objects (talk)
Orradre, J.; Blanco, P.M.; Madurga, S.; Mas, F.; Garcés, J.L.
The influence of mechanical streching on the ionization properties of LPEI (talk)
Mas, F.; Garcés, Blanco, P.M.; Madurga, S.; Carrera, M.

META: XV Congreso Español de Tratamiento de Aguas
Venue, A Coruña (Spain)
Celebration date (20/6/2024)
Biorrefinería Porcina: Avances en la Gestión Sostenible de Purines (talk)
Prado, A.; Serra-Toro, A.; Ventura, M.; Segura, Y.; Pariente, I.; Melero, J.A.; Martínez, F.; Astals, S.; Mas, F.; Dosta, J.; Puyol, D.
Operación a largo plazo de una membrana permeable al gas para la recuperación de nitrógeno de un efluente de fermentación acidogénica (poster)
Serra-Toro, A.; Peña-Picola, S. ; Barchello, F.; Astals, S.; Mas, F.; Dosta, J.

RHODES 2024: 11th International Conference on Sustainable Solid Waste Management
Venue, Rhodes (Greece)
Celebration date (19-22/6/2024)
Long-term performance of a gas-permeable membrane for nitrogen recovery of acidogenic fermentation effluenst (talk)
Serra-Toro, A.; Barchello, F.; Astals, S., Mas, F.; Dosta, J.

Personalized Health 2024
Venue, Zurich (Switzerland)
Celebration date (26/8/2024)
Insights from Immune-Metabolic Classification in Colorectal Cancer: Targeting Metabolic Vulnerabilities through drug repurposing (poster)
Madurga, S.; Marín, S.; Mas, F.; Maurel, J.; Cascante, M.

Swiss Metabolomics Society Annual Meeting
Venue, Basel (Switzerland)
Celebration date (29(/8/2024)
Distinctive metabolic colorectal cancer subtypes identified by multi-omics data integration. (poster)
Cascante, M.; Lopez-Blanco, D.; Foguet, C.; Tarrado-Castellarnau, M.; Centelles, J.J.; Madurga, S.; Marin, S.

46 Congreso de la Sociedad Española de Bioquímica y Biología Molecular
Venue, A Coruña (Spain)
Celebration date (3/9/2024)
Distinctive metabolic colorectal càncer subtypes identified by multiomics data integration (poster)
Marin, S.; Lopez Blanco, D.; Foguet, C.; Tarrado-Castellarnau, M.; Centelles, J.J.; Madurga, S.; Cascante, M.

Cancer Metabolism 2024
Venue, Bilbao (Spain)
Celebration date (8/10/2024)
Distinct Metabolic Signatures in Colorectal Cancer Unveiled Through Integrative multi-omics profiling (poster)
Cascante, M.; Lopez-Blanco, D.; Madurga, S.; Bori-Bru, B.; Perez-Leon, R.; Tarrado-Castellarnau, M.; Mas, F.; de Atauri, P.; Marin, S.
Multi-Omics and Genome-Scale Metabolic Models Highlight Metabolic Vulnerabilities Tied to FOLFOX Adaptations in Colorectal Cancer (poster)
López-Blanco, D.; Marin, S.; Foguet, C.; Tarrado-Castellarnau, M.; Bori-Bru, B.; Centelles, J.; de Atauri, P.; Madurga, S.; Cascante, M.

1er Congreso de la Sociedad Española de Bioinformática y Biología Computacional
Venue, Barcelona (Spain)
Celebration date (16/10/2024)
Distinct Metabolic Signatures in Colorectal Cancer Unveiled Through Integrative Multi-omics Profiling (poster)
López-Blanco, D.; Madurga, S.; Bori-Bru, B.; Pérez-León. R.; Tarrado-Castellarnau, M.; Mas, F.; de Atauri, P.; Marin, S.; Cascante, M.
Targeting metabolic vulnerabilities in colorectal càncer: insights from immune-metabolic classification (poster)
Madurga Díez, S.; Marín, S.; Mas, F.; Maurel, J.; Cascante, M.
Integrating multi-omics data into genome-scale metabòlic models identifies unique metabòlic vulnerabilities linked to the chemoresistance of FOLFOX chemotherapy in colorectal cancer (poster)
Cascante, M.; López-Blanco, D.; Madurga, S.; Bori-Bru, B.; Pérez-León. R.; Tarrado-Castellarnau, M.; Mas, F.; de Atauri, P.; Marin, S.

Mitochondria and Metabolism in Health and Disease. 10th Annual MetNet International Meeting
Venue, Barcelona (Spain)
Celebration date (24/10/2024)
Integrative Multi-Omics Profiling Reveals Distinct Metabolic Signatures in Colorectal Cancer (poster)
Cascante, M.; López-Blanco, D.; Madurga, S.; Bori-Bru, B.; Pérez- León, R.; Tarrado-Castellarnau, M.; Mas, F.; de Atauri, P.; Marín, S.
Multi-Omics and Genome-Scale Metabolic Models Highlight Metabolic Vulnerabilities Tied to FOLFOX Adaptations in Colorectal Cancer (poster)
López-Blanco, D.; Marín, S.; Foguet, C.; Tarrado-Castellarnau, M.; Bori-Bru, B.; Centelles, J.; de Atauri, P.; Madurga, S.; Cascante, M.

7th Iberian Carbohydrate Meeting
Sitges (Spain)
15-17/01/2024
Novel mechanisms of glycosyltransferases involved in protein glycosylation (Oral communication)
C. Rovira

JNCASR - CECAM Conference MD@60
Bangalore (India)
26-29/02/2024
QM/MM MD simulations of protein glycosylation reactions (Oral communication)
C. Rovira

NIC Days: Biomolecular Evolution, Function, and Assembly - Theory Meets Experiment
Juelich (Germany)
24-26/04/2024
The Functional Role of an N-glycan in the Human α-L-Iduronidase Is Mimicked by a LOOP in Bacterial Orthologues (Poster)
Q. Liao

15th Carbohydrate Bioengineering Meeting (CBM15)
Ghent (Belgium)
5-8/05/2024
QM/MM simulations of GT-mediated protein glycosylation reactions (Oral communication)
C. Rovira
Unraveling A4GALT mechanism and inhibit: towards a therapeutic approach for Fabry Disease (poster)
O. Vidal-Girones
Molecular mechanism of syn-acting mannuronan-specific PL7 alginate lyases (Flash presentation and Poster)
J.P. Rivas-Fernández

16th Bratislava Symposium on Saccharides
Smolenice Cabstle (Slovakia)
23-27/09/2024
Non-classical glycosylation mechanisms: a modelling approach (Plenary address)
C. Rovira

Computational chemistry across scales and disciplines: celebrating the 60th birthday of Ursula Röthlisberger.
CECAM, Lausanne (Switzerland)
1-3/10/2024
Discovering glycosylation mechanisms (Oral Communication)
C. Rovira
The role of the 2-OH interaction in the reaction mechanism of 1,3-1,4-β-glucanase (Poster)
A.Pepe

Innovative high-performance computing approaches for molecular neuromedicine.
Institute of Neurosciences and Medicine (INM). Forchungszentrum Julich (Germany)
5-8/11/2024
QM/MM simulation of protein glycosylation mechanisms (Online talk)
C. Rovira

Highlighting Organic Chemistry in Catalonia. Joint virtual symposium of the European Chemical Society (EuChemS) and the Catalan Society of Chemistry (SCQ)
Barcelona (Spain)
8/11/2024
Protein glycosylation mechanisms (Oral Communication)
C. Rovira

VII RSEQ Chemical Biology Group Meeting - ChemBioVII
Sevilla (Spain)
18-20/11/2024
Fundamental aspects of enzyme catalysis to inform biotechnology approaches (Plenary address)
C. Rovira
Unraveling the Mechanism of A4GALT and Insights into Adamantyl-galactoceramide Analogues: Towards a Therapeutic Approach for Fabry Disease (poster)
O. Vidal-Girones
The molecular mechanism of AmGH181: a recently discovered sialidase from Akkermansia muciniphila (poster)
M. Corbella

4th FUSION Frontiers in Photochemistry Conference
Dolce CampoReal Resort (Lisbon, Portugal)
10 Jul - 13 Jul 2024
THERMALLY-ACTIVATED DELAYED FLUORESCENCE PHOTOREDOX CATALYSTS IN SYNTHETIC ORGANIC CHEMISTRY (Invited Lecture)
B. Limburg

Young Investigator Awards
UCD Campus, Dublin, Ireland
5 July-6 July 2024
Mechanistic Implications in Cobalta-photoredox Catalysis for the Synthesis of Quaternary Carbons *(Invited Lecture)*
B. Limburg

Young Investigators Symposium, ACS Fall 2024
Denver, USA
18 August – 22 August 2024
Mechanistic Implications in Cobalt-photoredox Catalysis for the Synthesis of Quaternary Carbons *(Invited Lecture)*
B. Limburg

Summer School, German project SPP2080 "Catalysts and reactors under dynamic conditions for energy storage and conversion"
Barcelona (Spain)
16/10/2024
Approaching complexity of catalytic nanomaterials by DFT calculations (invited talk)
K.M. Neyman

Colloquium "Supported metal nano-particles and alloys for catalytic applications", 31st General Conference of the Condensed Matter Division of the European Physical Society
Braga (Portugal)
04/09/2024
How oxide supports affect transition-metal particles in catalytic nanomaterials (invited talk)
K.M. Neyman

Cluster of Excellence "Materials for Energy Conversion and Storage"
TU Wien, Vienna (Austria)
17/04/2024
How to give a good talk (invited talk)
K.M. Neyman

Conference of the COST Action 18234
Vienna (Austria)
03/04/2024
Approaching complexity of nanomaterials for catalysis by DFT modelling (invited talk)
K.M. Neyman

Cluster of Excellence "Materials for Energy Conversion and Storage"
TU Wien, Vienna (Austria)
20/03/2024
Computational modelling of bimetallic nanoparticles (invited talk)
K.M. Neyman

37th Workshop on Chemistry and Physics of Novel Materials
Schladming (Austria)
06/02/2024
Quantifying interface effects in catalytic nanomaterials combining DFT modelling and experiments (invited talk)
K.M. Neyman

4th Internat. Conference on Fundamentals and Applications of Cerium Dioxide in Catalysis
Portorož-Portorose (Slovenia)
19/09/2024
When platinum metal is not noble: Platinum-oxide clusters supported on ceria (talk)
K.M. Neyman, J. Quinlivan, P. Castro-Latorre, A. Bruix

Cluster-surface interactions for energy applications
Bernried, Germany,
9/04/2024
Modeling the response of supported particles to reaction conditions (invited talk)
A. Bruix

III JORNADA DELS INSTITUTS DE RECERCA PROPIS DE LA UB
Barcelona, Espanya
13/02/2024
Data Science i Machine Learning: una nova era per a la química computacional (invited talk)
A.Bruix

XIX Encuentro de Química Inorgánica de la Sociedad Chilena de Química
Hotel Santa Cruz, Santa Cruz (Chile)
20-23/10/2024
Shape and symmetry of coordination polyhedra in lanthanide compounds
P. Alemany

The Third International Process Intensification Conference (IPIC3)
Beijing (China)
28-31/May/2024
Structure and dynamics first principles simulations of CO_2 hydrogenation in Nickel/Cerium Oxide catalyst (invited talk)
P. Gamallo, X. Giménez, P. Lozano-Reis, R. Sayós.
CO_2 hydrogenation on modified zeolites from atomistic to fluid dynamics simulations (invited talk)
X. Giménez, P. Gamallo, M. Cánovas, R. Sayós

University of Concepción Summer School
Concepción (Chile)
8-12/Jan/2024
Química teórica aplicada a la resolución de problemas industriales (invited talk)
P. Gamallo

PhD Multidisciplinary Chemical Congress
Gijón (Spain)
14-15/Mar/2024
CO_2 hydrogenation on Ru encapsulated on silicalite: a multiscale study (talk)
M. A. Cánovas, R. Sayós, P. Gamallo

Workshop 2024 on Theoretical Chemistry and Computational Modelling
Tarragona (Spain)
3/Jun/2024
Silicalite-encapsulated Ru atoms: a multiscale study using DFT, MD and CFD (poster)
M. Cánovas, R. Sayós, P. Gamallo

Research Stays in Recognized Centers

Prof. Gerard Alonso
Universidad de Concepción, Concepción (Chile)
Pablo Gamallo Belmonte, UB
Jan 2024

Prof. Dr. Gianfranco Pacchioni
University of Milano Biccoca, Milano (Italy)
Néstor García-Romeral, University of Barcelona
February–May 2024

Prof. Dr. Kai S. Exner
University of Duisburg-Essen, Essen (Germany)
Ling Meng, University of Barcelona
February–May 2024

Günther Rupprechter
Technische Universität Wien, Vienna (Austria)
Konstantin Neyman, Dept. Ciència de Materials i Química Física
February-May 2024

Ijen Chen
Nxera Pharma UK Limited, Cambridge (United Kingdom)
Özge Ergün, University of Barcelona
March-May 2024

Prof. Mu Hua Huang
Beijing Institute of Technology (BIT), Beijing (China)
Prof. Josep Puigmartí Luis, Universitat de Barcelona
March-April 2024

António M. Baptista
Instituto de Tecnologia Química e Biológica, Lisboa (Portugal)
Renato Dias da Cunha, University of Barcelona
April-May 2024

Jaime Llanos & Sergio Conejeros
Departamento de Química de la Universidad Católica del Norte, Antofagasta (Chile)
Pere Alemany, Univ. Barcelona
May 2024

Dr. Michelle Long
Wanhua University, Yantay (China)
Pablo Gamallo Belmonte, UB
May 2024

Prof. Salvador Pané Vidal
ETH Zürich, Zürich (Switzerland)
Mr. Anh Tuan Ngo, Universitat de Barcelona
June 2024

Prof. Tania Patiño Padial
Eindhoven University of Technology, Eindhoven (Netherlands)
Prof. Josep Puigmartí Luis, Universitat de Barcelona
July 2024
Eindhoven University of Technology, Eindhoven (Netherlands)
Dr. Maria Guix Noguera, Universitat de Barcelona
July 2024

Dr. Denys Makarov

Helmholtz-Zentrum Dresden-Rossendorf, Dresden (Germany)
Prof. Josep Puigmartí Luis, Universitat de Barcelona
July 2024

Prof. Salvador Pané Vidal

ETH Zürich, Zürich (Switzerland)
Ms. Gemma Llauradó Capdevila, Universitat de Barcelona
September - Decembre 2024

Prof. Michele Parrinello

Instituto Italiano di Tecnologia (IIT), Genova (Italy)

José Pablo Rivas-Fernandez, Universitat de Barcelona (SQPBio group)

September-December 2024

Prof. Mu Hua Huang

Beijing Institute of Technology (BIT), Beijing (China)
Prof. Josep Puigmartí Luis, Universitat de Barcelona
October 2024

Prof. Zuobin Wang

Changchun University of Science and Technology (CUST), Changchun (China)
Prof. Josep Puigmartí Luis, Universitat de Barcelona
November 2024

Prof. Claudio Villani

Sapienza Università di Roma, Roma (Italy)
Prof. Josep Puigmartí Luis, Universitat de Barcelona
December 2024

Participation in Competitive Funded Research Projects

ALLODD - Allostery in Drug Discovery.
Carles Curutchet, Xavier Barril & Jordi Juárez, Universitat de Barcelona
H2020-MSCA-ITN-2020 Project 956314, 2021-2025
Financing entity (EU)
Amount: 454,049.76 €

Estudio computacional multiescala de la conversión catalítica de gases de efecto invernadero y la producción de hidrógeno mediante zeolitas funcionalizadas.
Pablo Gamallo Belmonte / Ramon Sayós Ortega, Universitat de Barcelona
PID2022-138180OB-I00, 01/09/2023 - 31/08/2026
Ministerio de Ciencia e Innovación - Programa CTQ - PN de Ciencias y Tecnologías Químicas
Amount: 118.750,00 €

Institut de Química Teòrica i Computacional (IQTC)
Eliseo Ruiz Sabin, Universitat de Barcelona
CEX2021-001202-M, 01/01/2023 - 31/12/2026
Ministerio de Ciencia e Innovación
Amount: 2.000.000,00 €

Introducció de la impressió 3D en assignatures impartides per la Secció d'Enginyeria Química a la Facultat de Química
Alberto Cruz Alcalde, Universitat de Barcelona
2023PID-UB/019, 01/01/2024 - 31/12/2026
Amount: 2.400,00 €

Simulació aplicada a l'aprenentatge actiu en assignatures d'Enginyeria Química i Química Analítica
Roger Bringue Tomas, Universitat de Barcelona
2023PEDC-QUI/001, 01/10/2023 - 01/10/2025
Tipus Projecte Programa PEDC - Projectes Estratègics Docents de Centre (PEDC)
Amount: 0,00 €

Computational Materials Science Laboratory (CMSL) / Laboratori de Ciència de Materials Computacional
Francesc Illas Riera, Universitat de Barcelona
2021 SGR 00079, 01/01/2022 - 30/06/2025
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR) - Tipus Grup Programa SGRC - Ajuts de Suport als Grups de Recerca de Catalunya (SGR)
Amount: 60.000,00 €

A paradigm shift for the future's thermal management devices through radical innovation in new materials and additive manufacturing (ThermoDust)
Sergi Dosta Parras / Camila Barreneche Guerisoli, Universitat de Barcelona
101046835, 01/11/2022 - 31/10/2026
Unió Europea - Tipus Projecte Programa 9P3EIC - HE - European Innovation Council Període
Amount: 656.796,00 €

Doctorat Industrial 'Captura directa de CO2 del aire'. Empresa: Recam Laser SL
Jordi Bonet Ruiz / Xavier Giménez, Universitat de Barcelona
2022 DI 0024, 08/06/2022 - 07/06/2025
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)
Amount: 33.960,00 €

Grup d'Estructura Electrònica (GEE)
Pedro Alemany Cahner, Universitat de Barcelona
2021 SGR 00286, 2022-2025.
Financing entity: Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR).
Amount: 40.000€

Ajuts extraordinaris per a grups de Recerca de la Facultat de Química de la UB, que no han obtingut finançament en la convocatòria 2022 del Ministerio de Ciencia e Innovación
Jesús Jover Modrego, Universitat de Barcelona
2575QU02072030, 2024-2024.
Facultat de Química, Universitat de Barcelona.
Amount: 2.500€

Rational design of small molecules able to stabilize transient protein-protein complexes of oncological interest
PI: Jordi Juárez-Jiménez, Universitat de Barcelona
PID2023-148468OB-I00, 2024-2027
Financing entity: MINECO
Amount: 106.250,00€

Charting New Paths: First-in-class TREX2 inhibitors for psoriasis and dermatitis
PI: Concepció Soler Prat, Universitat de Barcelona
2024 PROD 00106, 2024-2026
Financing entity: GENCAT
Amount: -

Ajut per a la intensificació de les activitats de transferència
PI: Carles Galdeano Cantador, Universitat de Barcelona
JUB2024A 600457, 2024-2025
Financing entity: UB
Amount: -

Modelling the interplay between structure and spectroscopy in biosystems.
Carles Curutchet, Universitat de Barcelona
PID2020-115812GB-I00, 2021-2024
Financing entity (MINECO)
Amount: 96,800 €

Computational Biology and Drug Design.
F. Javier Luque, Universitat de Barcelona
2021SGR00671, 2022-2025
Financing entity (GENCAT)
Amount: 40,000 €

Structural and dynamic bases for the modulation of energy transfer and photosynthetic efficiency in biosystems.
Carles Curutchet, Universitat de Barcelona
PID2023-151584NB-I00, 2024-2027
MICIU
Amount: 112,500 €

Explorando nuevas estrategias en enfermedades víricas y tuberculosis: Plasticidad conformacional, resistencia a mutaciones y modificación química pseudoirreversible.
F. J. Luque, Universitat de Barcelona
PID2020-117646RB-I00, 2021-2024
MINECO
Amount: 170610€

Nuevas herramientas terapéuticas frente a influenza y tuberculosis: Diseño de fármacos guiado por multivalencia, cribado basado en hidrofobobicidad y modificación covalente.
F. J. Luque, Universitat de Barcelona
PID2023-147942OB-I00, 2024-2027
MINECO
Amount: 132500€

Método iterativo experimental y computacional para modular péptidos bioactivos de leptina para diseñar nuevas estrategias terapéuticas contra la enfermedad de Alzheimer
C.Pubill-Ulldemolins, C.Estarellas, Universitat de Barcelona
PID2022-142623OA-I00, 2023-2026
MINECO
Amount: 106250€

Computationally Driven Tuning Up of Novel Bidimensional MXene Catalysts for Greenhouse Gases Reduction and Hydrogen Generation (GREEN2DCAT).
Francesc Viñes and Carme Sousa, Universitat de Barcelona
PID2021-126076NB-I00, 2022-2025
Financing entity: MICIU-AEI
Amount: 169.400 €

Atom-Dispersed Catalysts for the Thermo-Photo Valorization of CO_2 (AD-TPCO2)
Francesc Illas and Francesc Viñes, Universitat de Barcelona
TED2021-129506B-C22, 2023-2025
Financing entity: MICIU-AEI
Amount: 169.510 €

Excited States Dynamics of TiO_2 Nanostructures: Towards Engineering Enhanced Photocatalytic Activity Under Sunlight (EXCILIGHT)
Ángel Morales-García, Universitat de Barcelona
PID2020-115293RJ-I00, 2022-2025
Financing entity: MICIU-AEI
Amount: 45.530 €

European Cooperation in Science & Technology (COST)
Francesc Illas WG1 PI, Universitat de Barcelona
COST Action IG18234, 2024-2025
Financing entity: COST
Amount: 125.000 €

Nanoscaled Hybrid Magnetic Materials: New Key Actors Unleashing Solar Overall Water Splitting
Marta Estrader Bofarull, Universitat de Barcelona
2023 CLIMA 00022, 2024-2026
Financing entity: AGAUR
Amount: 251.640 €

Juan de la Cierva Program
Moses Abraham Bokinala, Francesc Viñes Host, Universitat de Barcelona
FJC2021-047213-I, 2023-2024
Financing entity: MICIU-AEI
Amount: 64.800 €

Pep-SICO: Peptide-based systems as artificial compartments to diagnose non-Alzheimer Tauopathies diseases;
Mohit Kumar (Universitat de Barcelona), Co-Ordinator: Prof. Ana Pina.
RL001994, 2024-2027
Financing entity**:** La Caixa health 2024, La Caixa foundation.
Amount: 999,994 €.

Materiales blandos químicamente alimentados con funciones similares a sistemas vivos
Mohit Kumar, Universitat de Barcelona
PID2021-126244NA-I00, 2022-2025,
Financing entity**:** Proyectos De Generación De Conocimiento 2021(MINECO)
Amount: 75,020 €.

Chemically Fueled Soft Materials with Life-like Functions
Mohit Kumar, Universitat de Barcelona
RYC2021-035016-I, 2023-2027,
Financing entity**:** Ayudas para contratación Ramón y Cajal 2021, MINECO,
Amount: 40,000 €

Interacciones no-covalentes en macromoléculas de ADN no-naturales y clústeres de boro
Jordi Poater, Universitat de Barcelona
PID2022-138861NB-I00, 2023-2026
Financing entity: MINECO
Amount: 125.000€

Suport a Grups de Recerca
Mercè Deumal Solé, Universitat de Barcelona
2021 SGR 00354, 2022-2024
GENCAT
40.000 €

Autoensamblaje controlado por combustible de materiales supramoleculares porosos funcionales bajo condiciones de reacción-difusiónfuera del equilibrio (FUELSUPMAT-RD).
A. Sorrenti, Universitat de Barcelona
PID2023-151814NB-I00 (Proyectos de Generación de Conocimiento 2023) 2024-2027
Ministerio de Ciencia e Innovación
Amount: 101.250 €

Autoensamblaje disipativo de materiales supramoleculares porosos basados en cajas metal-orgánicas (DISSPORMAT).
A. Sorrenti, Universitat de Barcelona
CNS2023-145154 (Consolidación Investigadora 2023) 2024-2026
Ministerio de Ciencia e Innovación
Amount: 199.583 €

Síntesis y crecimiento controlado de estructuras metal-orgnaicas porosas con tecnologías microfluidicas
J. Puigmartí Luis, Universitat de Barcelona
PID2020-116612RB-C33 *2021-2024*
Ministerio de Ciencia e Innovación
Amount: 177.500 €

Magnetoelectric 3D printing technology - the revolution of actuatable composites (EVA),
J. Puigmartí Luis, Universitat de Barcelona
101047081 *(EIC Pathfinder Open 2021) 2022-2026*
European Union
Amount: 629.875 €

ChemInFlow Group (Chemistry In Flow and Nanomaterials Synthesis Group)
J. Puigmartí Luis, Universitat de Barcelona
SGR-Cat 2021 SGR 00270 *2022-2025*
AGAUR
Amount: 36.000 €

Towards a decarbonized chemical industry: enhancing the performance of Cu2O nanocatalysts in CO2 electrolyzers
Roc Matheu Montserrat and J. Puigmartí-Luis is a member of the team, Universitat de Barcelona
CLIMA – AGAUR - RN002882, 2024-2026
Agencia de Gestión de Ayudas Universitarias y de Investigación (AGAUR) - (GENCAT)
Amount: 208.395,00 €

European metal-organic framework network: combining research and development to promote technological solutions' (EU4MOFs).
Prof. Stefan Wuttke, Prof. Puigmartí-Luis (Management Committee) (UB)
CA22147, 2023 - 2027
COST Action (EU)
680.000 €

MAgnetically steerable wireless Nanodevices for the tarGeted delivery of therapeutIc agents in any vascular rEgion of the body (ANGIE)
Prof. Salvador Pané (ETH Zurich), Prof. J. Puigmartí-Luis is the project leader at UB
402185 (952152), 2021 – 2024 (EU)
European Commission; FET PROACTIVE; Call: H2020-EIC-FETPROACT-2019
4,000,000.00 €

Accepted in 2024 but starting in 2025

High-throughput ultrasound-based volumetric 3D printing for tissue engineering (SONOCRAFT)
Prof. J. Puigmartí-Luis, UB
101187842 – SONOCRAFT, 2025 – 2029 (EU)
European Commission, HORIZON-EIC-2024-PATHFINDEROPEN-01, (EIC Pathfinder Open 2024)
2.999.625,00 €

A Training Programme on 5R's implementation in the design, manufacturing and application of micro and nanorobotic platforms (GREENS)
Dr. Maria Guix Noguera, UB
101169173 — GREENS, 2025 – 2029 (EU)
HORIZON-MSCA-2023-DN-01-01, MSCA Doctoral Networks 2023
4.031.589,60 €

Identificación de los subtipos metabólicos de cáncer colorrectal para el desarrollo de medicina personalizada.
IP: Marta Cascante, Universitat de Barcelona
PID2020-115051RB-I00, 2021-2024
Financing entity (MINECO)
Amount: 350.900

Grup de Bioquímica Integrativa.
IP: Marta Cascante, Universitat de Barcelona
2021 SGR 00350, 2022-2025
Financing entity (GENCAT))
Amount: 60.000

Integración de membranas permeables al amoníaco y bioreactores anaeróbicos de membrana para producir fertilizantes y biogás a partir de aguas residuales de alta carga.
IPs: Joanda Dosta, Sergi Astals, Universitat de Barcelona
TED2021-132422B-I00, 2022-2025
Financing entity (MINECO)
Amount: 195.500

Una estrategia integral para valorizar residuos procedentes de granjas porcinas mediante la producción de recursos valiosos para el sector alimentario.(VALPIG4FOOD).
IP: Daniel Puyol, Universitat Rey Juan Carlos (Madrid)
TED2021-129595B-I00, 2022-2025
Financing entity (MINECO)
Amount: 184.000

Uso de nuevas técnicas computacionales de modelamiento a multiescala para la determinación de los mecanismos de adsorción de ácidos húmicos a lixiviados de microplásticos.
IP: Haruna L. Barazorda, Universitat Católica Santa María (Arequipa, Perú)
VRINVFMP003-POP-092022, 2023-2025
Financing entity (UCSM, Arequipa, Perú)
Amount: 25.000

Integrated Targeting Bacterial DNA Replication: Investigating Elvitegravir's Inhibition of Topoisomerase IV.
IP: Sergio Madurga, Universitat de Barcelona
BCV-2024-2-0015
, 2024-2024
Financing entity (Red española de Supercomputación)
Amount:

Integrated Analysis of Metabolic Pathways, Patient Classfication, and Knock-Out Strategies in Colorectal Cancer.
IP: Sergio Madurga, Universitat de Barcelona
BCV-2024-2-0017, 2024-2024
Financing entity (Red española de Supercomputación)
Amount:

Modelización de la interacción metabólica en el microambiente del cáncer colorectal: Gemelos digitales metabólicos para el diseño de nuevas terapias combinadas.
IP: Marta Cascante, Universitat de Barcelona
PID2023-150539OB-I00, 2024-2028
Financing entity (MINECO)
Amount: 350.000

Utilització d'una nova membrana hidrofòbica/hidrofílica per a la recuperació i valorització del Namoniacalde dejeccions porcines (FERTIAMONIA),
IP: Francesc Mas, Universitat de Barcelona
ACC_2023_EXP_SIA002_13_0000705, 2024-2026
Financing entity (GENCAT)
Amount: 58.027

Diseño in silico de un novedoso compuesto teranóstico para la leishmaniasis basada en la química del anfitrión-huesped utilizando la Base de Datos de Productos Naturales del Perú (PeruNPDB) y hospederos macrocíclicos.
IP: Haruna L. Barazorda, Universitat Católica Santa María (Arequipa, Perú)
PE501088204-2024-PROCIENCIA, 2024-2027
Financing entity (CONCYTEC, Perú)
Amount: 25.000

A PREDicitive signature in rectal cancer, treated with total neoadjuvant therapy, to increase the accuracy of WATCH and WAIT strategy.
IPs: Joan Maurel, Marta Cascante, Pedro R. Rodrigues, Universitat de Barcelona
EHD24PI02, 2024-2026
Financing entity (CIBER-cáncer)
Amount: 197.500

Molécula activadora de la señalización de kras oncogénico como terapia dirigida contra el cáncer colorectal.
IP: Nieves Agell Jane, Universitat de Barcelona
NBME, PDC2022-133653-I00, 01/12/2022- 31/08/2025 extended
W0122 - Ministerio de Ciencia e Innovación
149.500,00 €

SGRC - Ajuts de Suport als Grups de Recerca de Catalunya (SGR)
IP: Marta Cascante Serratosa, Universitat de Barcelona
2021 SGR 00350/ 01/01/2022- 30/06/2025
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)
60.000,00 €

Master Evaluation and Material Transfer Agreement
Investigadores responsables: Nieves Agell Jane / Eduardo Garrido Sagarzazu / Jaime Rubio Martinez / Bara Abuasaker / Sonia Brun Lozano / Montserrat Jaumot Pijoan / Marta Vilaplana Saiz / Maria Pujol Dilme
KNOW-Contractes d'explotació de know-how. Royalties o derivats de cesió de llicència/patent/know-how. 06/06/2023-05/06/2027
Entidad Financiadora: ValiRx PLC

Mimicking the reaction transition state of carbohydrate-active enzymes with superacids
Carme Rovira, Universitat de Barcelona; Sebastien Thibadeau, CNRS-Université de Poitiers; Jesus Jimenez Barbero, CICbioGUNE, Bilbao
IRP GLYCOMIMIC, 01/02/2022-31/12/2027
French National Research Agency (ANR).
Amount:

Activity-Based Profiling of Glycoprocessing Enzymes for Human Health and a Sustainable Society
Carme Rovira, Universitat de Barcelona; Gideon J. Davies, University of York; Hermen Overkleeft, University of Leiden
ERC-2020-SyG-951231, 01/06/2021-31/05/2027
European Research Council. Grant agreement No 951231
Amount: Total grant 9.057.250 €. Amount corresponding to UB (C. Rovira): 1.984.750 € (indirect costs).

Computer simulation of catalytic mechanisms in glycoprocessing enzymes by means of QM/MM molecular dynamics techniques
Carme Rovira, Universitat de Barcelona
PID2020-118893GB-100, 01/09/2021-31/08/2024
I+D project of the Spanish Ministry of Science and Innovation (MICINN)
Amount: 120.000,00 € (145.200,00 €, indirect).

Estructura i funció en macromolècules
Carme Rovira, Universitat de Barcelona; Ignasi Fita, CSIC
2021SGR-00680, 01/01/2022-30/06/2025
AGAUR (Generalitat de Catalunya)
Amount: 60.000€

GLYCOprotein N-glycosylation from non-life to eukaryotes: a Doctoral Network to expand the knowledge on a ubiquitous posttranslational modification of proteins (GLYCO-N)
Co-PI: Carme Rovira, Universitat de Barcelona; Coordinator: Antonio Molinaro, University of Naples
HORIZON-MSCA-2022-DN-01-01 Proposal ID 101119499, 01/02/2024-30/01/2027
Horizon MSCA
Amount: 2.724.364,80 € (full consortium), 251.971,20 € (UB-C. Rovira).

Computer simulation of the molecular basis of substrate recognition and catalysis in glycoprocessing enzymes
Carme Rovira, Universitat de Barcelona
PID2023-147939NB-I00, 01/09/2024-31/08/2027
I+D project of the Spanish Ministry of Science, Innovation and Universities (MICIU)
Amount: 150.000,00 € (187.500,00 €, indirect)

Equipamiento Científico Técnico (FlowNMR),
J.F. Sanguesa
EQC2024-008712-P,
MICIU
€ 582 608, as 'supporter' and author of the scientific part

Computational modelling of complex materials for advanced technologies
P. Alemany, K. Neyman, Universitat de Barcelona
PID2021-128217NB-I00, 2022-2025
MCIUN
108900€

Development and application of grand canonical global optimization methods assisted by machine learning
A. Bruix, Universitat de Barcelona
PID2022-140120OA-I00, 2023-2026
MCIUN
100,000 €

Excellence in colloid and interface research & innovations for better quality of life
K. Neyman (PI for UB), Universitat de Barcelona
Networking project "EXTREME", 2021-2024
Bulgarian Ministry of Education and Science
0€

Salvador de Madariaga grant
K. Neyman, Universitat de Barcelona
PRX22/00367, 2024
Ministerio de Universidades, Spain
11580€

Grant 2023 CLIMA
M. Mas Torent, ICMAB
2023 CLIMA 00064, 2024-2025
Agència de Gestió d'Ajuts Universitaris i de Recerca (AGAUR)
360000€

Solar Spectral Conversion based on Luminescent Lanthanide Complexes of Isoquinoline ligands. Luminescent down-shifting layers and Luminescent Solar Concentrators to enhance photovoltaic efficiency in crystalline silicon cells.
J. Llanos, U. Católica del Norte (Antofagasta, Chile)
Fondecyt Regular 1220159, 2023-2026
Agencia Nacional de Investigación y Desarrollo (Chile)
Amount:

Patent or Mark Application

Vacancies in carbon-based 2D layers
Ideaded, S.L.; Stefan T Bromley, Ibério de PR Moreira, Miquel Lopez-Suarez, Genis Lleopart,; Fundació Institució Catalana de Recerca i Estudis Avançats (ICREA)
Application number: EP24382481.0 (european patent application)

Contracts with Industry

Serveis en química computacional.
2020-2024
F. J. Luque
Pharmacelera

Title. Fabricació i optimització de pel·lícules fines per a dispositius electrònics avançats
Titular/s: Natalia Salvat Lozano (Industrial PhD), Prof. Josep Puigmartí Luis (academic responsable), Jemish Mahendrabhai Parmar (Industry responsable)
IDEADED

Characterization of the immunometabolic actions of benfo-oxythiamine (B-OT) and analogs in human macrophages: An approach to understanding the role of these drugs on tumor-associated macrophages (TAM).
IPs: Marta Cascante, Sílvia Marín, Universitat de Barcelona
Financing entity (Benfovir AG, Germany), 2024-2025
Amount: 99.940,50

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i Computacional
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